

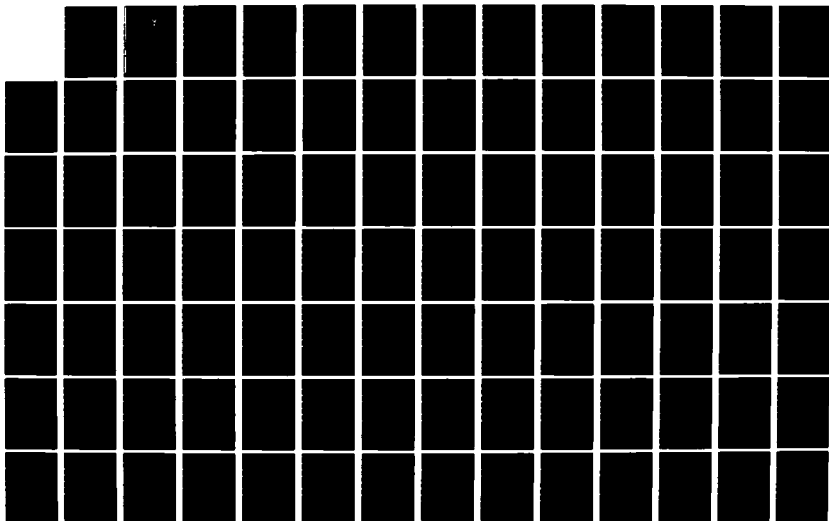
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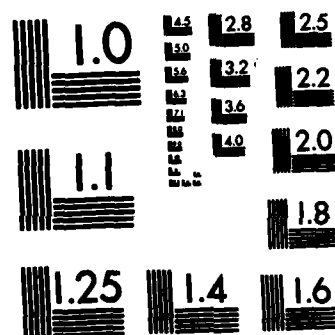
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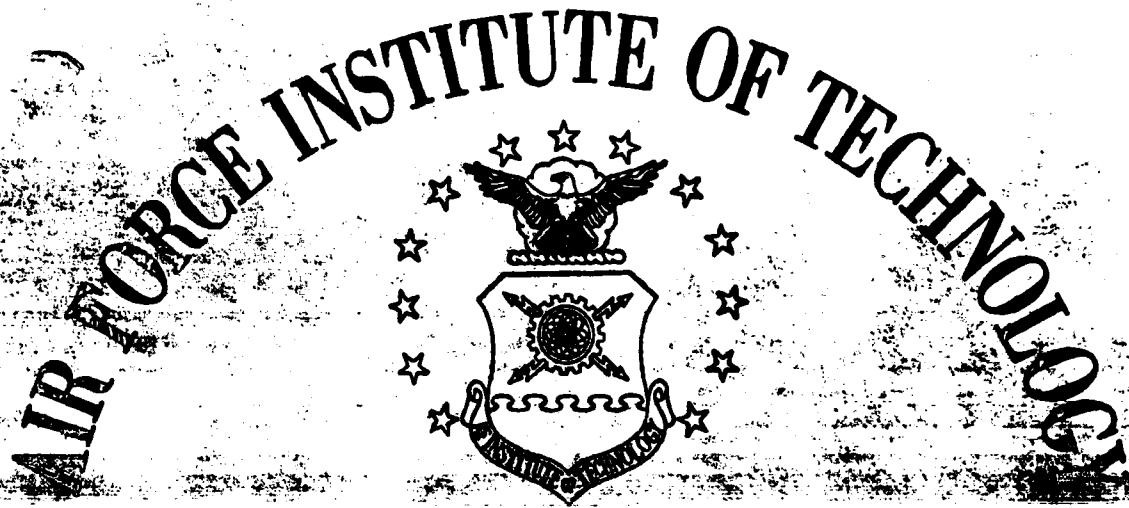
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UNITED STATES AIR FORCE

ACCURACY OF FINITE DIFFERENCE METHODS
FOR SOLUTION OF THE TRANSIENT
HEAT CONDUCTION (DIFFUSION) EQUATION

THESIS

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T. Sidney Chivers, Jr.
Capt USA/OrdC

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ACCURACY OF FINITE DIFFERENCE METHODS
FOR SOLUTION OF THE TRANSIENT
HEAT CONDUCTION(DIFFUSION) EQUATION

THESIS

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology

Air University

In Partial Fulfillment of the
Requirements for the Degree of
Master of Science

by

T. Sidney Chivers, Jr., B.S.

Capt

USA/OrdC

Graduate Nuclear Engineering

January 1983

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Preface

Earlier in this study, the emphasis was on understanding the occurrence of oscillatory instabilities in finite difference approximations for two-dimensional transient heat conduction(diffusion). The Peaceman-Rachford alternating direction implicit (ADI) finite difference method (FDMTH) was of special interest. As the computer programs for the various FDMTHs were debugged and data began to accumulate, the emphasis shifted to the accuracy of the FDMTHs. The Crank-Nicholson implicit FDMTH proved to be the most accurate of the methods considered and the Peaceman-Rachford ADI FDMTH the least accurate.

Dr. Bernard Kaplan's guidance and encouragement throughout this study were always timely and effective. Special thanks are due Dr. W. Kessler of the Air Force Materials Laboratory for sponsoring this research project. I am especially indebted to my wife, Madalene, and our three children who have survived my master's thesis.

T. Sidney Chivers, Jr.

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Abstract

↓
The two-dimensional transient heat conduction (diffusion) equation was solved using the fully explicit, fully implicit, Crank-Nicholson implicit, and Peaceman-Rachford alternating direction implicit (ADI) finite difference methods (FDMTHs). The general stability condition for the same FDMTHs was derived by the matrix, coefficient, and a probabilistic method. The matrix, coefficient, and probabilistic methods were found to be equivalent in that each lead to the same general stability condition. Oscillatory behavior of the fully explicit FDMTH was as predicted by the general stability condition. Though the Crank-Nicholson implicit and the Peaceman-Rachford ADI FDMTHs were expected to be unconditionally stable, unstable oscillations were observed for large sizes of time step. For large numbers of time steps and sizes of time steps for which all FDMTHs considered are stable, the Crank-Nicholson implicit FDMTH is the more accurate. ←

I. Introduction

Background.

Finite difference methods are useful in obtaining solutions for engineering problems involving partial differential equations that cannot be solved in closed form. Because finite difference methods approximate the true solution, their competent use requires an understanding of discretization errors and the stability condition. The discretization error is the combined effect of round-off and truncation due to the "limitation on the number of significant figures carried by a computer" (2:20) and the truncation of higher order Taylor series terms in developing the finite difference approximations of partial differentials (2:20), respectively. The stability condition defines parameter regions in which the finite difference method remains stable for large numbers of time steps. The coefficient method (15,16,12:283), the matrix method (20:60-68), and the Fourier method (19) are the more common methods of deriving the stability condition. A probabilistic method of deriving the stability condition is suggested by the work of Kaplan (10).

Problem Statement.

The primary objectives of this study were to understand instability in finite difference methods and be able to predict when oscillatory behavior would occur. Secondary objectives were to compare the various methods of deriving the stability condition, and compare finite difference methods on the basis of discretization error and stability.

Scope.

This study was limited to two-dimensional transient heat conduction(diffusion) in a rectangular region. The finite difference methods considered were the fully explicit, fully implicit, Crank-Nicholson implicit, and Peaceman-Rachford alternating direction implicit. The matrix, coefficient, and probabilistic methods of deriving the stability condition were considered.

General Approach.

Computer programs were developed to solve the two-dimensional transient heat conduction(diffusion) problem by either the fully explicit, fully implicit, Crank-Nicholson implicit, or Peaceman-Rachford alternating direction implicit finite difference method. The thermodynamic and mathematical aspects of the stability of finite difference methods were researched. The stability condition for the general two-dimensional finite difference approximation of transient heat conduction(diffusion) was derived by the matrix, coefficient, and probabilistic methods. Computer programs developed were run for selected time increments and nodal array sizes to develop data for comparison of finite difference methods, and to assess the validity of the stability condition derived for the general finite difference method.

Sequence of Presentation.

Finite difference methods are discussed in the next section. The matrix methods used are described in Section III. The theory of stability analysis is detailed in Section IV. Computer methods and other procedures used are described in Section V. Results are summarized in Section VI with graphic results appended.

Acronyms.

Two acronyms will be used throughout the remainder of this thesis. FDMTH(s) will represent finite difference method(s), and ADI will represent alternating direction implicit. These acronyms are necessary for brevity. Using these acronyms, the Peaceman-Rachford alternating direction implicit finite difference method becomes the Peaceman-Rachford ADI FDMTH.

II. Transient Heat Conduction(Diffusion) by Finite Differences

The two-dimensional transient heat conduction (diffusion) problem considered in this study is described by the following initial-boundary value problem.

$$\frac{\partial T}{\partial t} = \alpha \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] \quad (1a)$$

$$T(0,y,t) = T(1,y,t) = T(x,0,t) = T(x,1,t) = 0 \quad (1b)$$

$$T(x,y,0) = \sin \pi x \sin \pi y \quad (1c)$$

where T is for temperature, α is the thermal diffusivity, x and y are spatial dimensions, and t is for time. The analytic solution, derived at Appendix A, is

$$T(x,y,t) = \exp[-\alpha(m^2\pi^2 + n^2\pi^2)t] \sin(m\pi x) \sin(n\pi y) \quad (1d)$$

In the following, the two-dimensional finite difference approximation of transient heat conduction(diffusion) is developed from two basic difference equations, the first forward difference and the second central difference. Error analysis is discussed in the final sub-section.

The General Finite Difference Approximation.

Approximating the time derivative in equation (1) by a first forward difference and the two spatial derivatives by second central differences, the finite difference approximation of two-dimensional transient heat conduction(diffusion) becomes

$$\begin{aligned} & \frac{T(i,j,k+1) - T(i,j,k)}{\Delta t} = \\ & \frac{\alpha [T(i+1,j) - 2T(i,j) + T(i-1,j)]}{(\Delta x)^2} \\ & + \frac{\alpha [T(i,j+1) - 2T(i,j) + T(i,j-1)]}{(\Delta y)^2} \end{aligned} \quad (2)$$

where the subscripts i , j , and k are used to identify the node location and time step. Figure 1 depicts a spatial domain discretized by imposing a 5 by 5 array of nodes over the domain so that, for equation (2), $i = 0, 1, 2, \dots, 5-1$ and $j = 0, 1, 2, \dots, 5-1$. For a general m by n nodal array, $i = 0, 1, 2, \dots, m-1$ and $j = 0, 1, 2, \dots, n-1$.

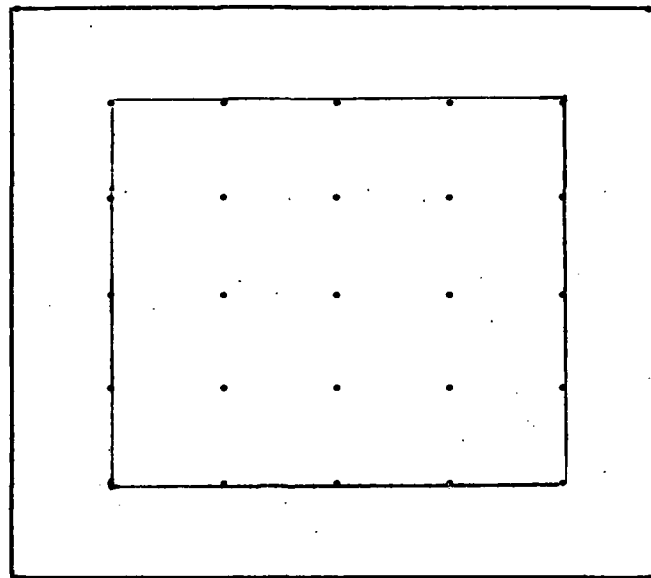


Figure 1. A 5 by 5 Nodal Array Imposed over the Domain of a Square Surface

To simplify notation, a common practice is to use nodal labels that indicate the locations of nodes relative to the node (i, j) as illustrated in Figure 2 where

$$T_E \equiv T(i+1, j) \quad (3)$$

$$T_W \equiv T(i-1, j) \quad (4)$$

$$T_N \equiv T(i, j-1) \quad (5)$$

$$T_S \equiv T(i, j+1) \quad (6)$$

$$T_P \equiv T(i, j) \quad (7)$$

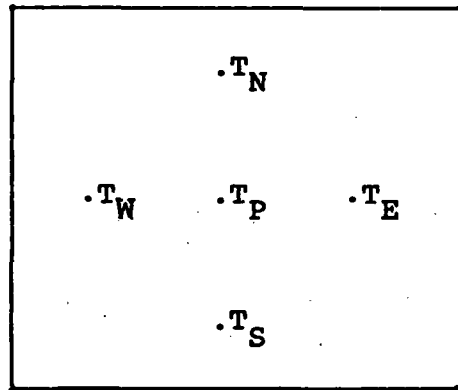


Figure 2. Relative Labelling of Nodes

Equation (2) now simplifies to

$$\begin{aligned} \frac{T_P^{k+1} - T_P^k}{\Delta t} &= \frac{\alpha \Delta t}{(\Delta x)^2} [T_E - 2T_P - T_W] \\ &+ \frac{\alpha \Delta t}{(\Delta y)^2} [T_N - 2T_P - T_S] \end{aligned} \quad (8)$$

The temperatures on the right side of equation (2) represent a mean temperature between time steps (15:28),

$$T_e = f_e T_e^{k+1} + (1-f_e) T_e^k \quad (9)$$

where f_e is some weighting factor.

From equations (8) and (9), the general two-dimensional FDMTH for transient heat conduction(diffusion) becomes

$$\begin{aligned}
 T_P^{k+1} - T_P^k = & \\
 & \frac{\alpha \Delta t}{(\Delta x)^2} \left[f_E T_E^{k+1} + (1-f_E) T_E^k + f_W T_W^{k+1} + (1-f_W) T_W^k \right. \\
 & \quad \left. - 2f_{P_{EW}} T_P^{k+1} - 2(1-f_{P_{EW}}) T_P^k \right] \\
 & + \frac{\alpha \Delta t}{(\Delta y)^2} \left[f_N T_N^{k+1} + (1-f_N) T_N^k + f_S T_S^{k+1} + (1-f_S) T_S^k \right. \\
 & \quad \left. - 2f_{P_{NS}} T_P^{k+1} - 2(1-f_{P_{NS}}) T_P^k \right] \quad (10)
 \end{aligned}$$

Figure 3 indicates the relative locations of the temperatures in equation (10). Values of f_e can be varied to reduce equation (10) to a specific finite difference method. Table 1 lists values of f_e for the fully explicit, fully implicit, Crank-Nicholson implicit, and Peaceman-Rachford ADI FDMTHs.

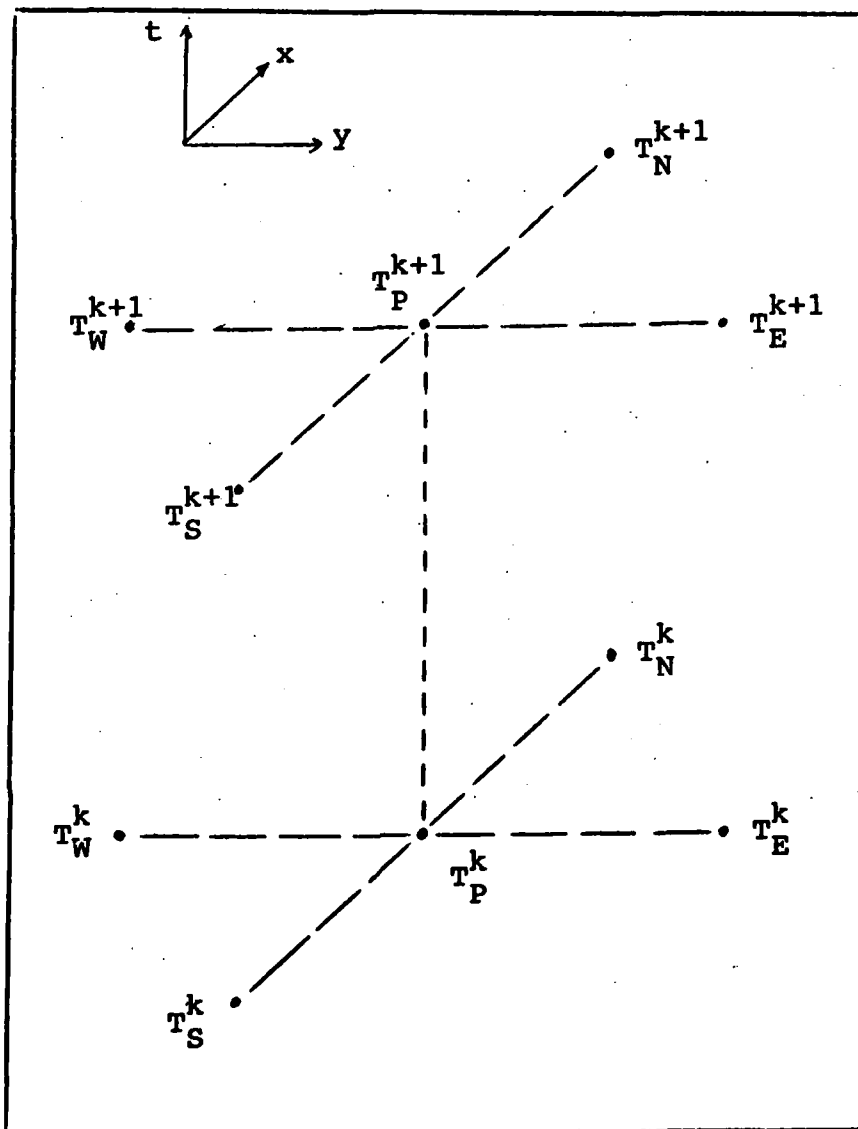


Figure 3. Relative Position of Nodes, or Temperatures, of the Generalized Two-dimensional Finite Difference Approximation of Transient Heat Conduction (Diffusion)

Table 1 <u>Weighting Factors for the Generalized</u> <u>Finite Difference Approximation of</u> <u>Transient Heat Conduction (Diffusion)</u>						
FDMTH	f_E	f_W	$f_{P_{EW}}$	f_N	f_S	$f_{P_{NS}}$
Fully Explicit	0	0	0	0	0	0
Fully Implicit	1	1	1	1	1	1
Crank-Nicholson Implicit	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Peaceman-Rachford ADI						
for Odd Time Steps	0	0	0	1	1	1
for Even Time Steps	1	1	1	0	0	0

Fully Explicit FDMTH.

The two-dimensional fully explicit FDMTH is explicit in both spatial dimensions. This FDMTH assumes nodal temperatures for time t prevail until time $t + \Delta t$ (15:56). From equation (10) and Table 1, the equation for the fully explicit FDMTH for transient heat conduction(diffusion) is

$$\begin{aligned} T_P^{k+1} - T_P^k &= \frac{\alpha \Delta t}{(\Delta x)^2} (T_E^k - 2T_P^k + T_W^k) \\ &+ \frac{\alpha \Delta t}{(\Delta y)^2} (T_N^k - 2T_P^k + T_S^k) \end{aligned} \quad (11)$$

or

$$\begin{aligned} T_P^{k+1} &= \frac{\alpha \Delta t}{(\Delta x)^2} (T_E^k + T_W^k) + \frac{\alpha \Delta t}{(\Delta y)^2} (T_N^k + T_S^k) \\ &+ \left[1 - \frac{2\alpha \Delta t}{(\Delta x)^2} - \frac{2\alpha \Delta t}{(\Delta y)^2} \right] T_P^k \end{aligned} \quad (12)$$

Figure 4 is the mnemonic for the fully explicit FDMTH.

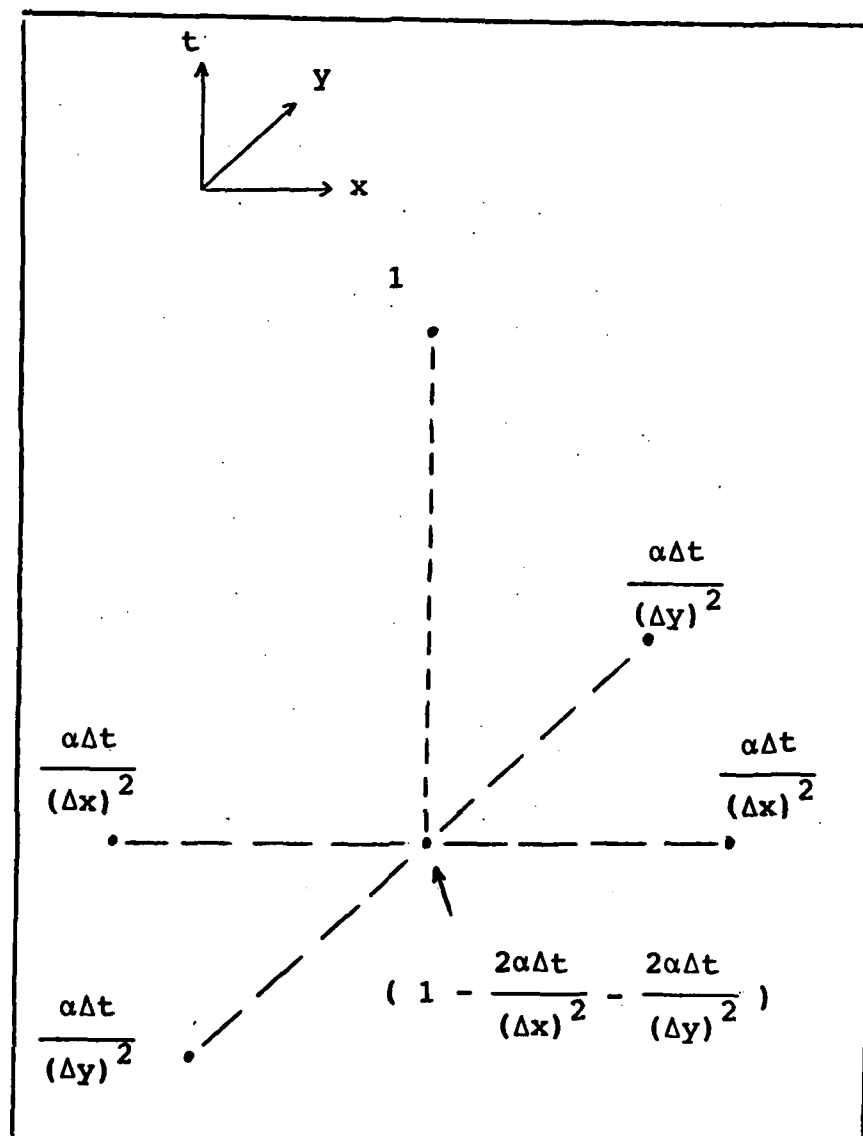


Figure 4. Mnemonic for the Fully Explicit FDMTH

Fully Implicit FDMTH.

The two-dimensional fully implicit FDMTH is implicit in both spatial dimensions. This FDMTH assumes nodal temperatures at time t change immediately to temperatures for time $t + \Delta t$ which prevail throughout the time step. From equation (10) and Table 1, the equation for the fully implicit FDMTH for transient heat conduction(diffusion) is

$$\begin{aligned} T_P^{k+1} - T_P^k &= \frac{\alpha \Delta t}{(\Delta x)^2} (T_E^{k+1} - 2T_P^{k+1} + T_W^{k+1}) \\ &+ \frac{\alpha \Delta t}{(\Delta y)^2} (T_N^{k+1} - 2T_P^{k+1} + T_S^{k+1}) \end{aligned} \quad (13)$$

or

$$\begin{aligned} &\left[1 + \frac{2\alpha \Delta t}{(\Delta x)^2} + \frac{2\alpha \Delta t}{(\Delta y)^2} \right] T_P^{k+1} \\ &- \frac{\alpha \Delta t}{(\Delta x)^2} (T_E^{k+1} + T_W^{k+1}) - \frac{\alpha \Delta t}{(\Delta y)^2} (T_N^{k+1} + T_S^{k+1}) \\ &= T_P^k \end{aligned} \quad (14)$$

Figure 5 is the mnemonic for the fully implicit FDMTH.

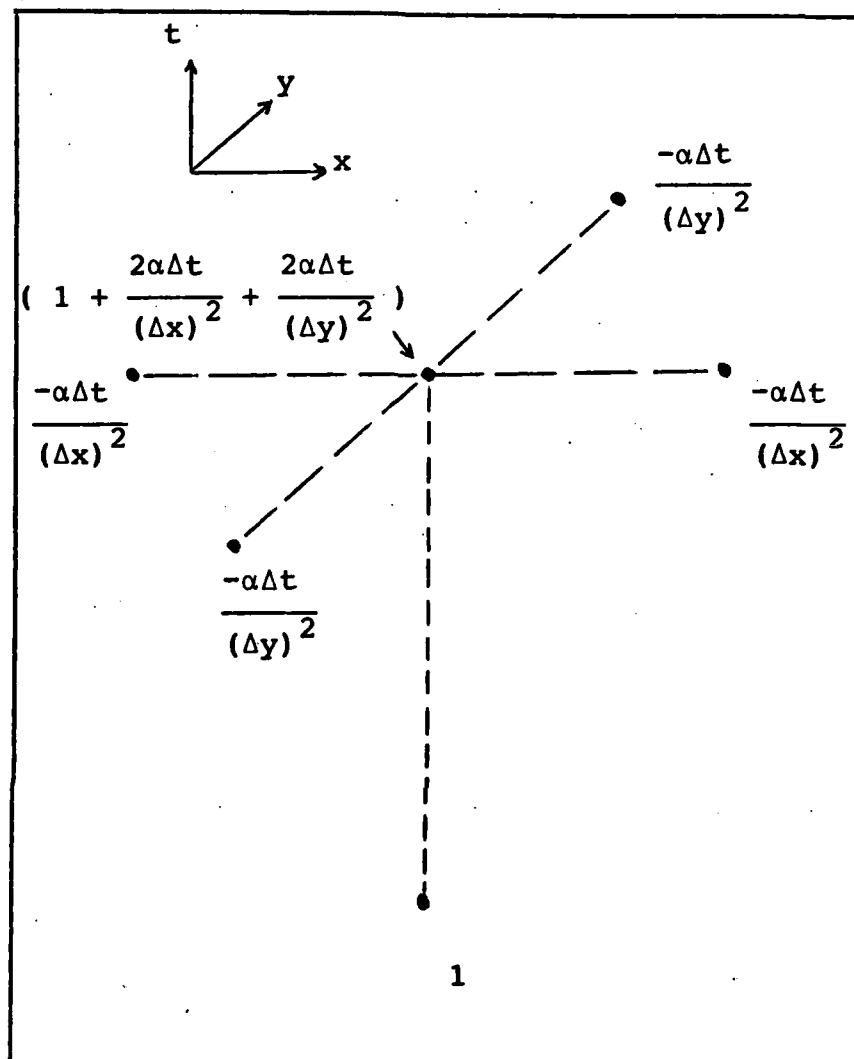


Figure 5. Mnemonic for the Fully Implicit FDMTH.

Crank-Nicholson Implicit FDMTH.

The two-dimensional Crank-Nicholson FDMTH assumes nodal temperatures change linearly from their value at time t to their value at time $t + \Delta t$. From equation (10) and Table 1, the equation for the Crank-Nicholson implicit FDMTH for transient heat conduction(diffusion) is

$$\begin{aligned} & \left[1 + \frac{\alpha \Delta t}{(\Delta x)^2} + \frac{\alpha \Delta t}{(\Delta y)^2} \right] T_P^{k+1} \\ & - \frac{\alpha \Delta t}{(\Delta x)^2} (T_E^{k+1} + T_W^{k+1}) - \frac{\alpha \Delta t}{(\Delta y)^2} (T_N^{k+1} + T_S^{k+1}) \\ & = \left[1 - \frac{\alpha \Delta t}{(\Delta x)^2} - \frac{\alpha \Delta t}{(\Delta y)^2} \right] T_P^k \\ & + \frac{\alpha \Delta t}{(\Delta x)^2} (T_E^k + T_W^k) + \frac{\alpha \Delta t}{(\Delta y)^2} (T_N^k + T_S^k) \end{aligned} \quad (15)$$

Figure 6 is the mnemonic for the Crank-Nicholson implicit FDMTH.

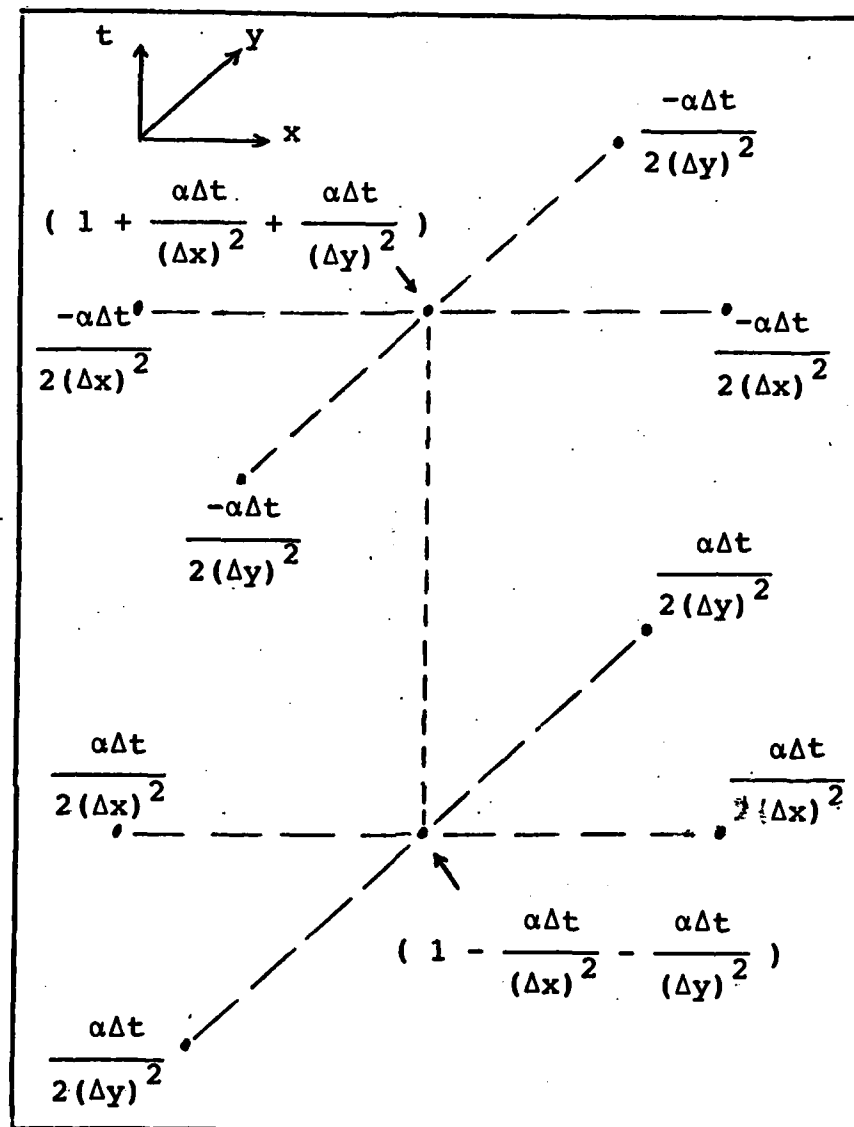


Figure 6. Mnemonic for the Crank-Nicholson Implicit FDMTH

Peaceman-Rachford ADI FDMTH.

The Peaceman-Rachford ADI FDMTH is a two step method. In the first step, nodal temperature changes are implicit with respect to one spatial dimension and explicit with respect to the other. In the second time step, the explicit/implicit roles of the two spatial dimensions are reversed. From equation (10) and Table 1, the equations for the Peaceman-Rachford ADI FDMTH for transient heat conduction(diffusion) are

$$\begin{aligned} & \left[1 + \frac{2\alpha\Delta t}{(\Delta x)^2}\right]T_P^{2k+1} - \frac{\alpha\Delta t}{(\Delta x)^2}(T_E^{2k+1} + T_W^{2k+1}) \\ &= \left[1 - \frac{2\alpha\Delta t}{(\Delta y)^2}\right]T_P^{2k} + \frac{\alpha\Delta t}{(\Delta y)^2}(T_N^{2k} + T_S^{2k}) \end{aligned} \quad (16)$$

and

$$\begin{aligned} & \left[1 + \frac{2\alpha\Delta t}{(\Delta y)^2}\right]T_P^{2k+2} - \frac{\alpha\Delta t}{(\Delta y)^2}(T_N^{2k+2} + T_S^{2k+2}) \\ &= \left[1 - \frac{2\alpha\Delta t}{(\Delta x)^2}\right]T_P^{2k+1} + \frac{\alpha\Delta t}{(\Delta x)^2}(T_E^{2k+1} + T_W^{2k+1}) \end{aligned} \quad (17)$$

Figures 7 and 8 are the mnemonics for the Peaceman-Rachford ADI FDMTH.

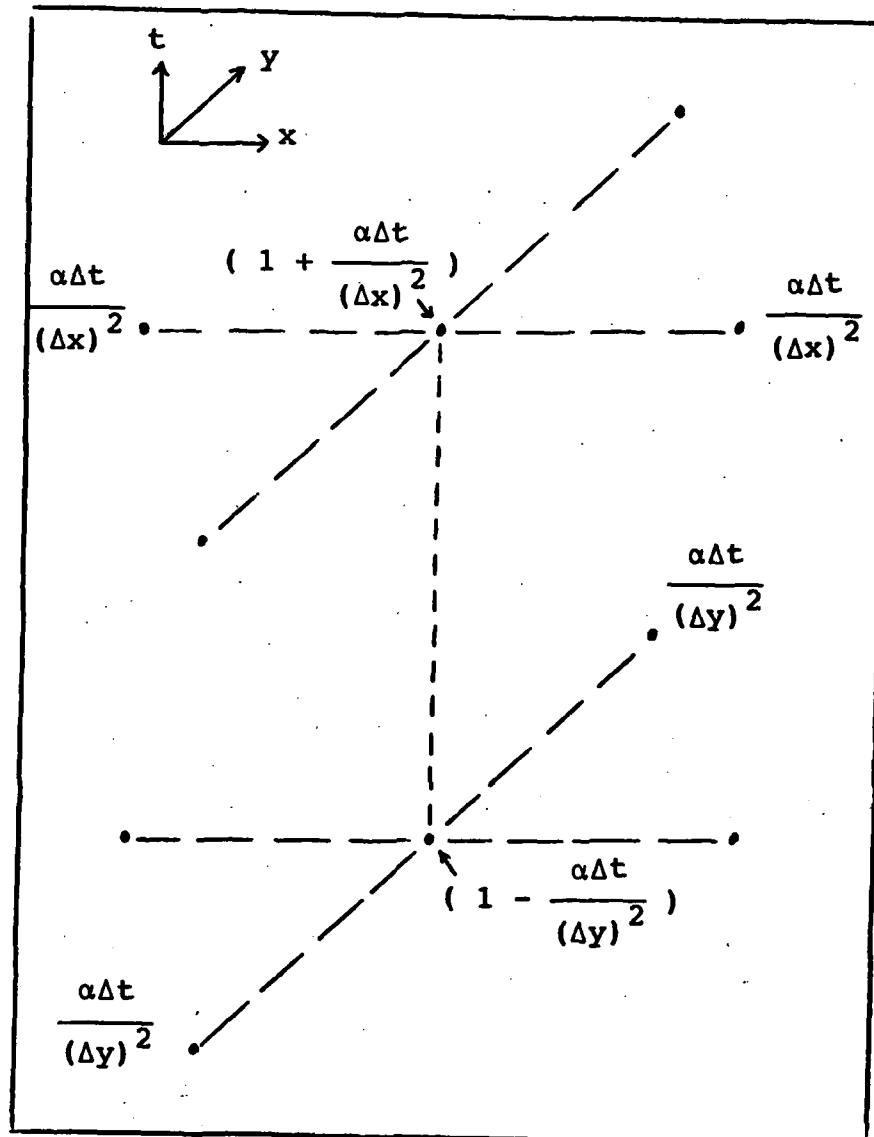


Figure 7. Mnemonic for the first step of the Peaceman-Rachford ADI FDMTH (Implicit in the x-direction)

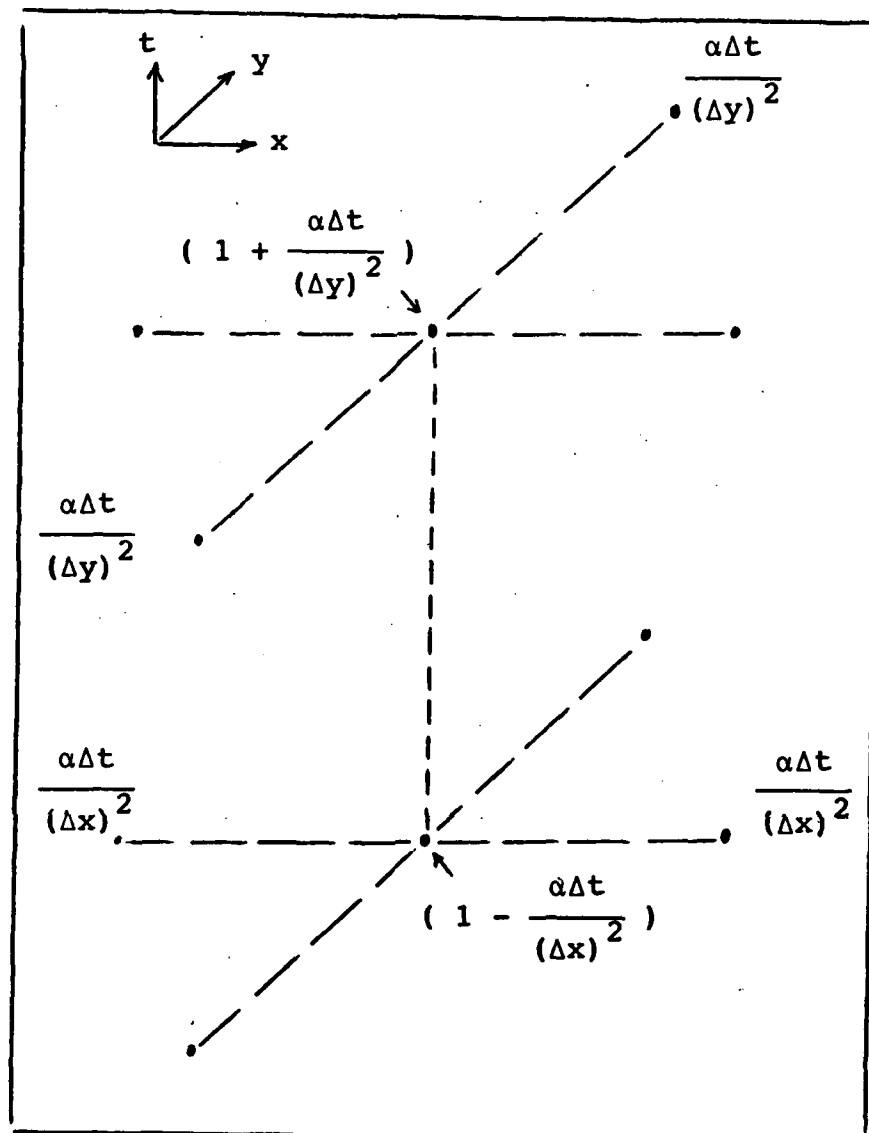


Figure 8. Mnemonic for the second step of the Peaceman-Rachford ADI FDMTH (Implicit in the y-direction)

Error Analysis.

The discretization error is the sum of the round-off error and the truncation error. The round-off error is dependent on the largest number of digits that can be represented in a computer's memory and the number of computations needed to obtain a solution. The truncation error is due to the truncation of higher order terms of the Taylor series representation of differentials in approximating the differentials by finite differences (2:20). Table 2 lists the order of truncation error expected with the fully explicit, fully implicit, Crank-Nicholson implicit, and Peaceman-Rachford ADI FDMTHs. In this study, the discretization error, ERR, is computed as the difference between the FDMTH and analytic solution temperatures, or

$$ERR = T_e^{k+1} - TR_e^{k+1} \quad (18)$$

where T_e^{k+1} is the FDMTH temperature of node e at time step k+1 and TR_e^{k+1} is the analytic solution temperature of node e at time step k+1.

Numerical stability, another aspect of error analysis of FDMTHs, is discussed in Section IV.

Table 2
Order of Truncation Error of
Selected Finite Difference Methods

FDMTH	Order of the Truncation Error
Fully Explicit	$\Delta t + (\Delta x)^2 + (\Delta y)^2$
Fully Implicit	$\Delta t + (\Delta x)^2 + (\Delta y)^2$
Crank-Nicholson Implicit	$(\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2$
Peaceman-Rachford ADI	
for Odd Time Steps	$\Delta t + (\Delta x)^2$
for Even Time Steps	$\Delta t + (\Delta y)^2$

III. Matrix Methods

Matrix methods are used to solve the simultaneous equations that result when applying any FDMTH that is partially or fully implicit, such as the fully implicit, Crank-Nicholson implicit, and Peaceman-Rachford ADI FDMTHs. The matrix equivalent of the general FDMTH equation, equation (10), is

$$\underline{A} \underline{T}^{k+1} = \underline{T}^k \quad (19)$$

where the coefficient matrix A is as shown in Figure 9. For example, the coefficient matrix for a 5 by 5 nodal array imposed over a square domain for the initial-boundary value problem (1), may be represented as

$$\begin{bmatrix} a & -b & 0 & -c & & & & \\ -b & a & -b & 0 & -c & & & \\ 0 & -b & a & 0 & 0 & -c & & \\ -c & 0 & 0 & a & -b & 0 & -c & \\ & -c & 0 & -b & a & -b & 0 & -c \\ & & -c & 0 & -b & a & 0 & 0 & -c \\ & & & -c & 0 & 0 & a & -b & 0 \\ & & & & -c & 0 & -b & a & -b \\ & & & & & -c & 0 & -b & a \end{bmatrix} \quad (20)$$

where the elements not shown are zero valued and

$$\begin{aligned}
 a &\equiv 1 + 2\alpha\Delta t[1-f_{P_{EW}}]/(\Delta x)^2 + 2\alpha\Delta t[1-f_{P_{NS}}]/(\Delta y)^2 \\
 &= a_{1,1} = a_{2,2} = \dots = a_{n,n}
 \end{aligned} \tag{21}$$

$$\begin{aligned}
 b &\equiv \alpha\Delta t(1-f_x)/(\Delta x)^2, \quad f_x = f_E = f_W \\
 &= a_{1,2} = a_{2,3} = \dots = a_{n-1,n} \\
 &= a_{2,1} = a_{3,2} = \dots = a_{n,n-1}
 \end{aligned} \tag{22}$$

$$\begin{aligned}
 c &\equiv \alpha\Delta t(1-f_y)/(\Delta y)^2, \quad f_y = f_N = f_S \\
 &= a_{1,M} = a_{2,M+1} = \dots = a_{n-M,n} \\
 &= a_{M,1} = a_{M+1,2} = \dots = a_{n,n-M}
 \end{aligned} \tag{23}$$

These type matrices are referred to as banded because all non-zero elements are within a band of n diagonals centered on the principal diagonal of the coefficient matrix. The width of the band is dependent on the array size used and the order in which the interior nodes are numbered. For example, if the interior nodes of a 8 by 4 nodal array are numbered from left to right and top to bottom, as in Figure 10, then the coefficient matrix is 13.

If the interior nodes of the same array are numbered top to bottom and left to right as in figure 11, then the bandwidth is 5. In general, the bandwidth, BW can be defined as

$$BW = 2m - 3 \quad (24)$$

for an m by n nodal array if the interior nodes are first numbered along the dimension corresponding to m.

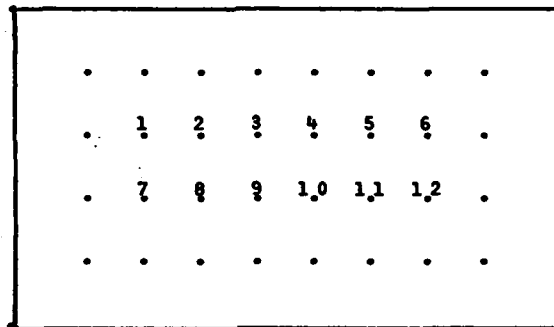


Figure 10. Interior Nodes of a
8 by 4 Nodal Array
Numbered Left to Right
and then Top to Bottom

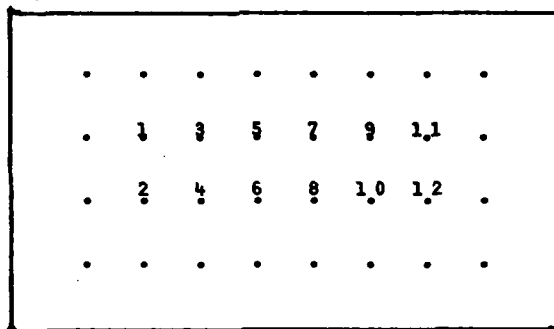


Figure 11. Interior Nodes of a
8 by 4 Nodal Array
Numbered Top to Bottom
and then Left to Right

If the coefficients in the two outer diagonals are all zero, as is the case for the Peaceman-Rachford ADI FDMTH, then the matrix is tridiagonal and a solution can be obtained by the Thomas method (3:46-48). An iterative process such as the method of Guass-Sidel (18:40-41) will solve the general form of the coefficient matrix. The Givens-Householder transformation can be used to reduce the general form to a tridiagonal coefficient matrix (14:85-115,22:901-914).

IV. Theory of Stability Analysis

Instability in finite difference methods can be considered caused by either violation of the first or second laws of thermodynamics (4), or use of an unstable numerical process. This study concentrates on the mathematical stability of FDMTHs. Oscillations of the same order of magnitude as the true solution are regarded as phenomenon characterizing marginal stability of FDMTHs. In the following, the matrix method (20:60-68), coefficient method (15,16,12:281-283), and the probabilistic method of deriving the stability condition will be described and two-dimensional forms presented.

Matrix Method.

A matrix equation for the general FDMTH for two-dimensional transient heat conduction(diffusion) is

$$\underline{A} \underline{T}^{k+1} = \underline{A}' \underline{T}^k \quad (28)$$

where the coefficient matrices \underline{A} and \underline{A}' are as described in Appendix A. Equation (28) can be rewritten as

$$[\underline{I} + (\underline{A} - \underline{I})] \underline{T}^{k+1} = [\underline{I} + (\underline{A}' - \underline{I})] \underline{T}^k \quad (29)$$

The stability condition is determined by examination of the eigenvalues of $[\underline{I} + (\underline{A}' - \underline{I})]$. The general FDMTH stability

condition for two-dimensional transient heat conduction (diffusion), derived at Appendix A, is

$$\kappa \equiv \alpha \Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \leq \frac{1}{2} \quad (30)$$

where $f_x = f_E = f_W$ and $f_y = f_N = f_S$. Table 1 depicts the values of f_e for the FDMTHs studied.

The Coefficient Method.

Descriptions of the coefficient method by Meyer (12:281-283) and by Patankar (15,16) differ only in symbology. Each considers the ratio, λ , of T^{k+1} to T^k as an indicator of stability. When λ is negative, the FDMTH is unstable. Table 3 gives the ranges of λ associated with the four types of stability of FDMTHs. Figure 12 depicts the finite difference stability curves for transient heat conduction(diffusion) in a square region with one interior node. The stability condition derived by the coefficient method is the same as the stability condition derived by the matrix method (See Appendix B).

Table 3

λ for the Four Possible Types of Behavior of FDMTHs
for Transient Heat Conduction(Diffusion)
in a Rectangular Region with One Interior Node
(20:282)

$\lambda > 1$	Steady, unbounded growth. T^{k+1} has the same sign as T^k and is larger in magnitude.
$1 > \lambda > 0$	Steady decay. T^{k+1} has the same sign as T^k and is smaller in magnitude.
$0 > \lambda > -1$	Stable oscillations. T^{k+1} has the opposite sign as T^k and is smaller in magnitude.
$\lambda < -1$	Unstable oscillations. T^{k+1} has the opposite sign as T^k and is larger in magnitude.

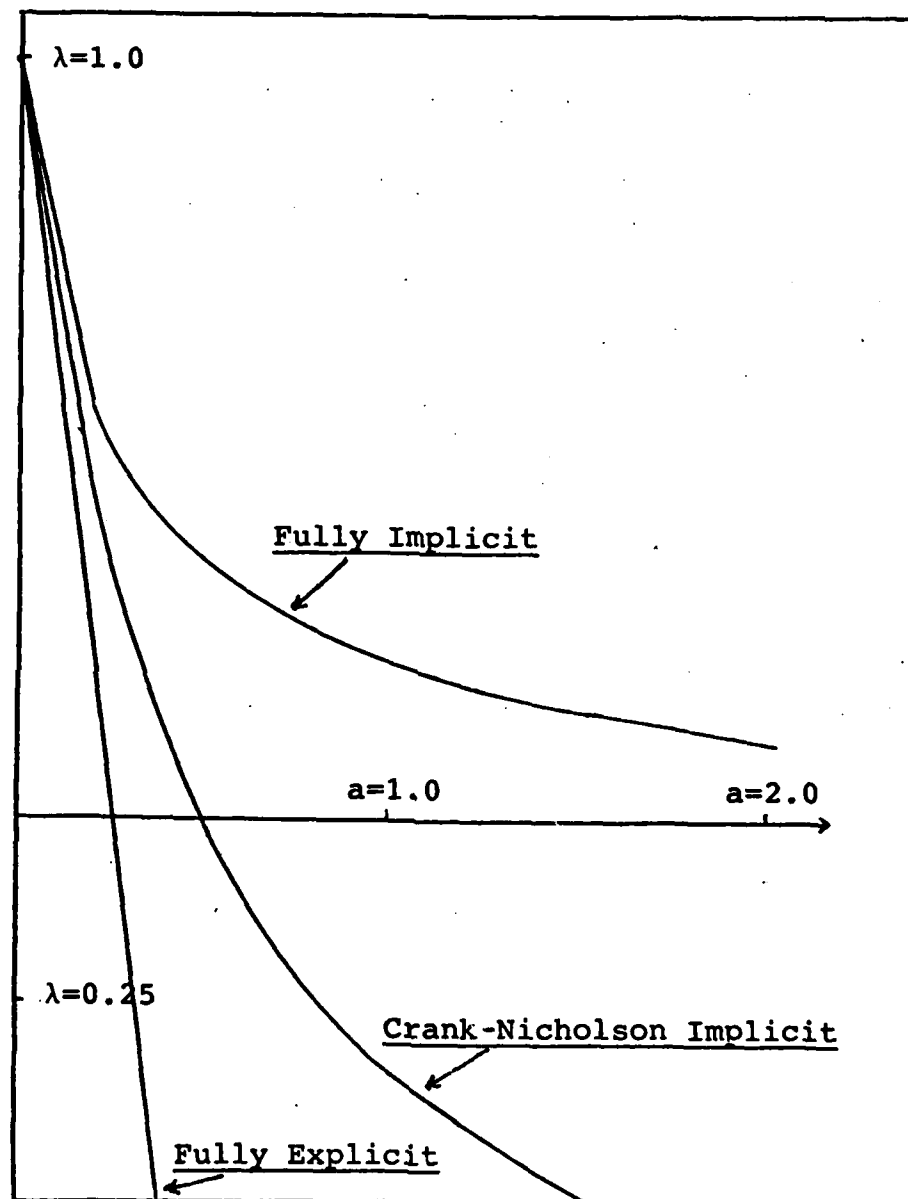


Figure 12. Finite Difference Stability Curves for Transient Heat Conduction (Diffusion) in a Square Region with One Interior Node

$$a = \frac{\alpha \Delta t}{(\Delta x)^2}$$

The Probabilistic Method.

The probabilistic method is suggested by the works of Kaplan (10), Haji-Sheikh and Sparrow (8), and Collins (5). By considering the coefficients of the general FDMTH to be probabilistic, a stability condition can be derived. The derivation of the stability condition by the probabilistic method for the general FDMTH for transient heat conduction(diffusion) is included as Appendix C. The stability condition derived by the probabilistic method is the same as the stability condition derived by the matrix and coefficient methods.

Summary.

All methods of stability analysis are equivalent in that each lead to the same stability condition,

$$\kappa \equiv \alpha \Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \leq \frac{1}{2} . \quad (33)$$

V. Procedures

Computer System.

The data in this study is from programs executed on the Harris 500 computer of the Air Force Institute of Technology.

Computer Programs.

Programs EXPLI, IMPLI, and PRADI were written for execution of the fully explicit, fully implicit and Crank-Nicholson implicit, and Peaceman-Rachford ADI FDMTHs, respectively. The Guass-Sidel method was used in IMPLI and the Thomas method was used in PRADI. Band storage, see Appendix F, was used to minimize memory requirements.

Error Analysis.

The four FDMTHs studied were compared on the basis of truncation error and stability. Truncation error was computed as the difference between the FDMTH temperature and the analytic temperature. The analytic temperature was computed from the analytic solution derived at Appendix A. Stability was studied by counting the number of oscillations about the true solution and noting occurrences of instability. Only data for those nodes along the diagonal from the northwest corner of the rectangular region to its center, see Figure 13, were considered.

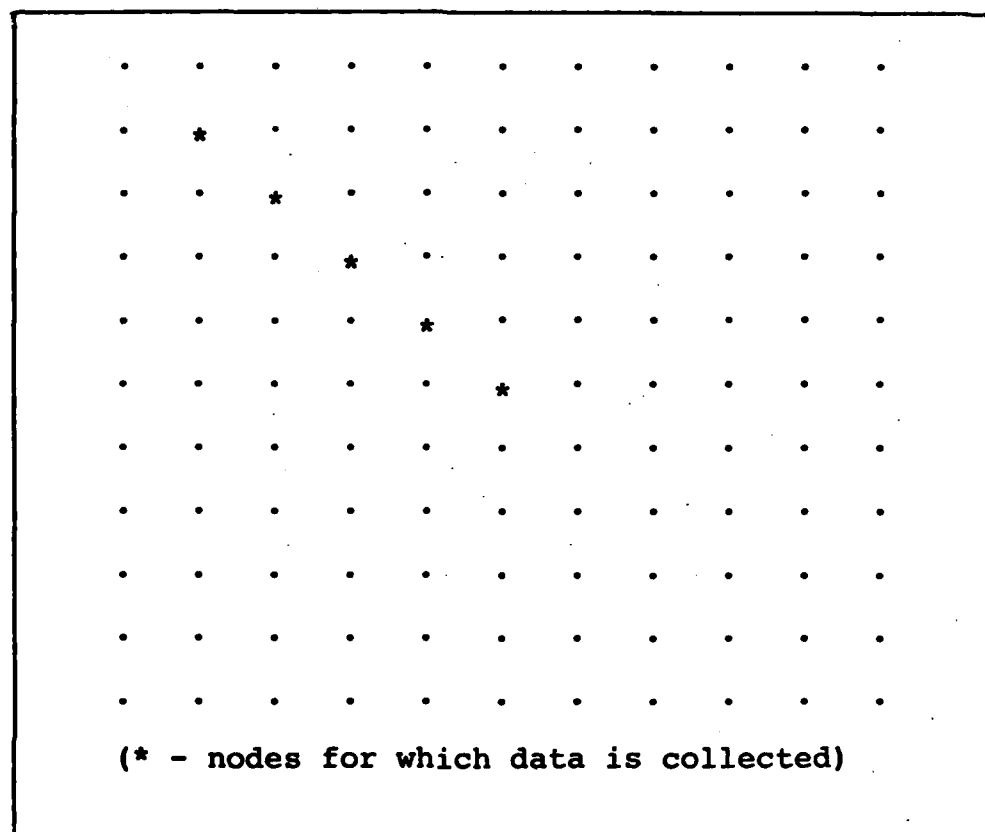


Figure 13. Nodes for which Data Would be Collected for a 11 by 11 nodal array.

Stability Conditions.

The stability condition for the general FDMTH for two-dimensional transient heat conduction(diffusion) was derived by the matrix method, the coefficient method, and the probabilistic method. The stability condition was used to select the program input parameters for execution of the various FDMTHs.

VI. Results

Most of the data collected in this study is at Appendix E. The following summarizes the results of this study.

Stability.

Applicability of the general stability condition, described in Section IV, was verified for the fully explicit and fully implicit FDMTHs. Though the Crank-Nicholson implicit and Peaceman-Rachford ADI FDMTHs were expected to be unconditionally stable, some unstable oscillatory behavior was observed for large time steps. Unstable oscillations for the fully explicit FDMTH were typically as depicted in Figure 14. Unstable behavior of the Crank-Nicholson implicit and Peaceman-Rachford ADI FDMTHs, for large time steps, is illustrated by figures 15 and 16 through 18, respectively. Edge effects, stable oscillations for nodes near corners, were observed for all FDMTHs. Edge effects for the fully implicit FDMTH are represented by Figure 19, where the number of oscillations for each node is represented by a number in the same relative position as the position of the node in the nodal array.

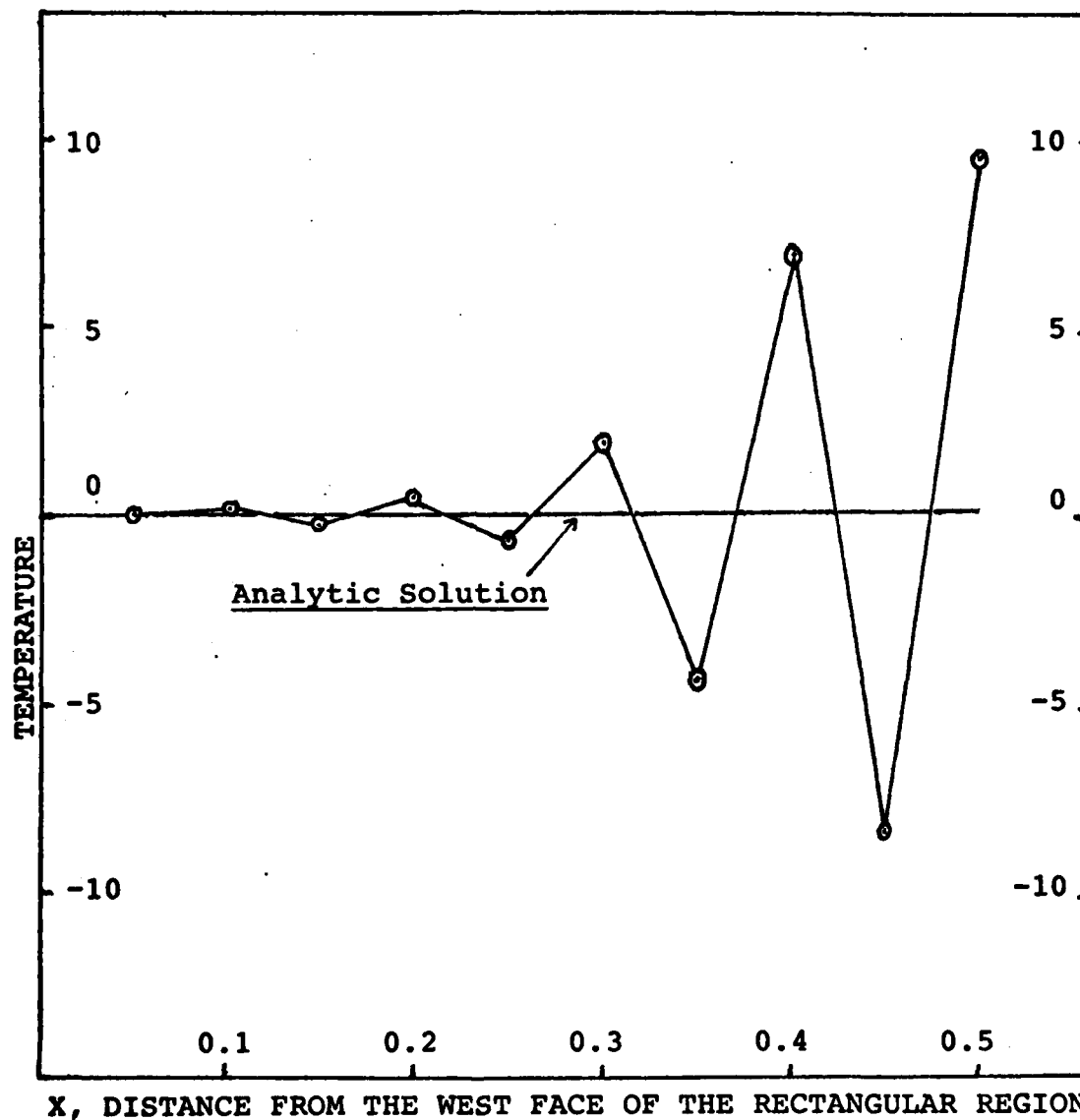
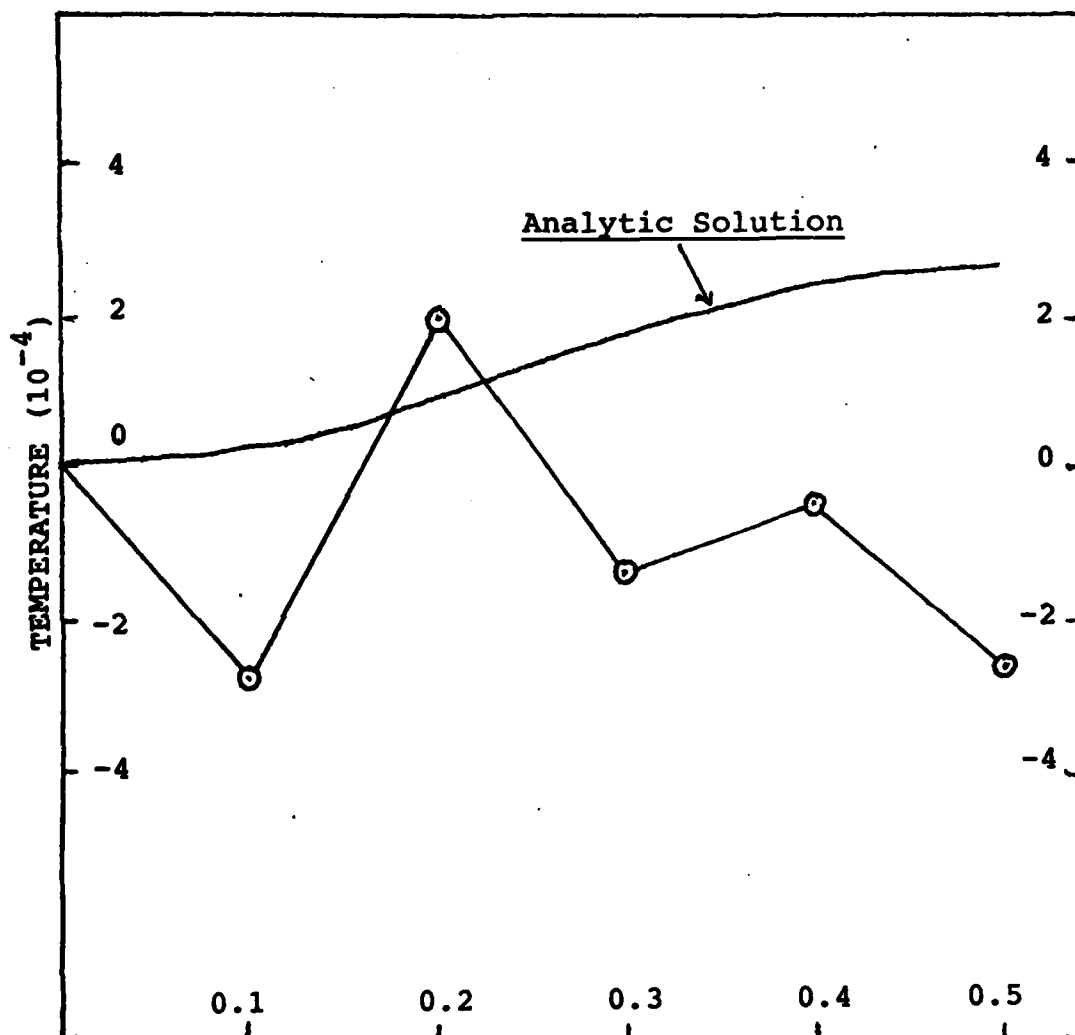


Figure 14. Unstable Oscillations for the Fully Explicit FDMTH for a 21 by 21 Nodal Array. Elapsed Time is 0.08. Time Step is 0.01. Number of Iterations is 8. $\kappa = 8$.



X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure 15. Unstable Oscillations for the Crank-Nicholson Implicit FDMTH for a 11 by 11 Nodal Array. Elapsed Time is 0.3. Time Step is 0.1. Number of Iterations is 3. $\kappa = 10$.

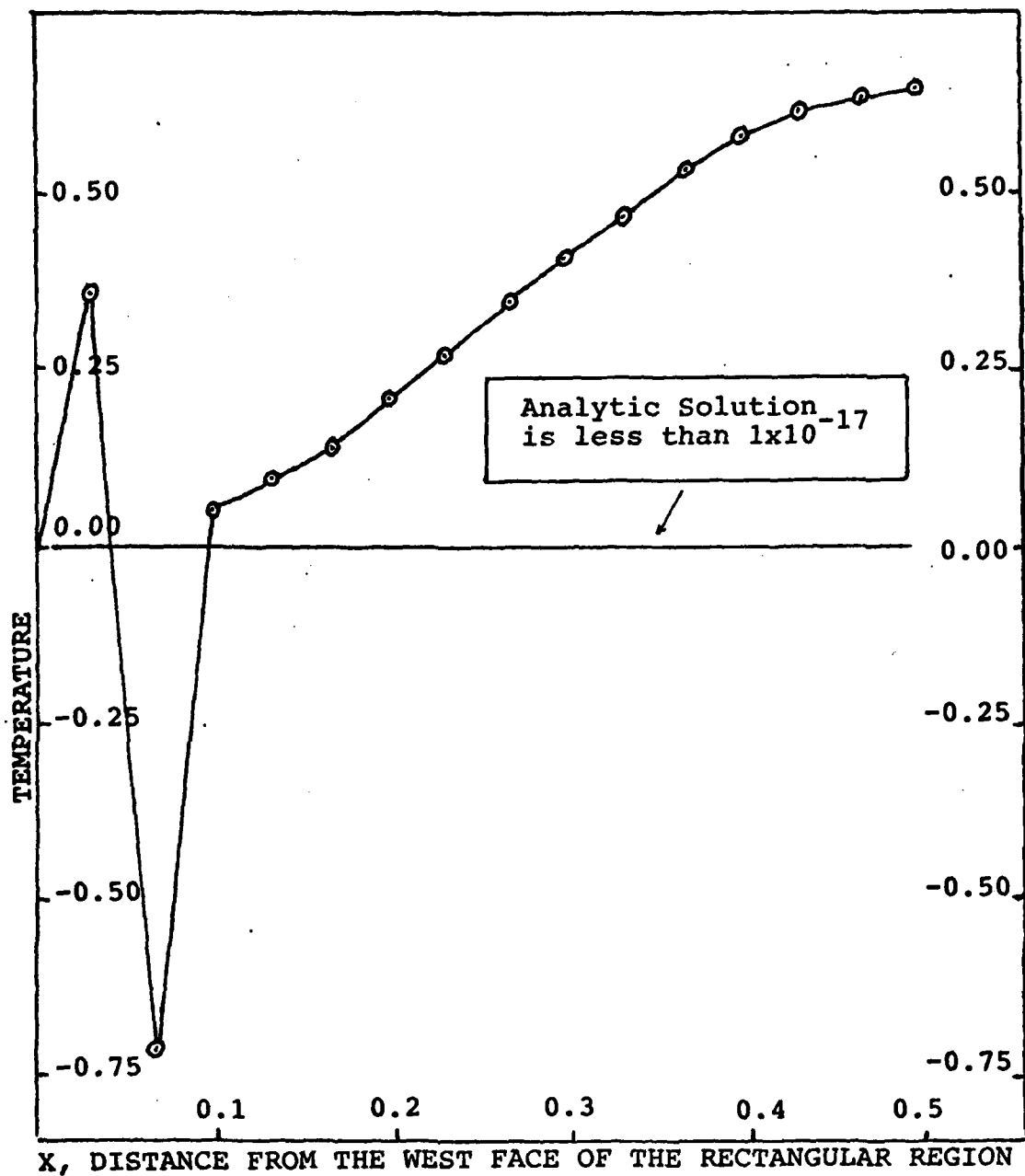


Figure 16. Unstable Oscillations for the Peaceman-Rachford ADI FDMTH for a 31 by 31 Nodal Array. Elapsed Time is 2. Time Step is 1. Number of Iterations is 2. $\kappa = 900$.

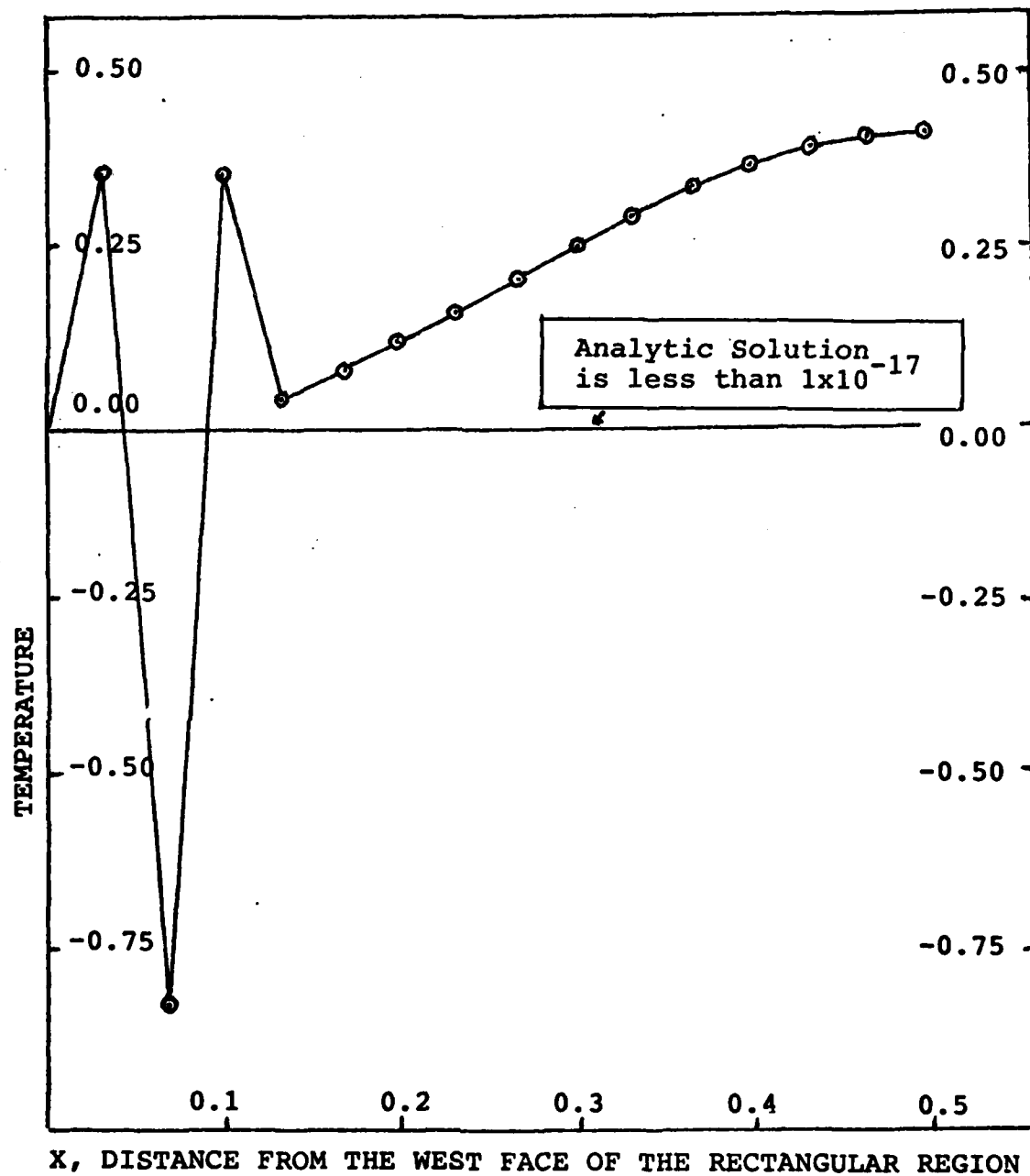


Figure 17. Unstable Oscillations for the Peaceman-Rachford ADI FDMTH for a 31 by 31 Nodal Array. Elapsed Time is 4. Time Step is 1. Number of Iterations is 4. $\kappa = 900$.

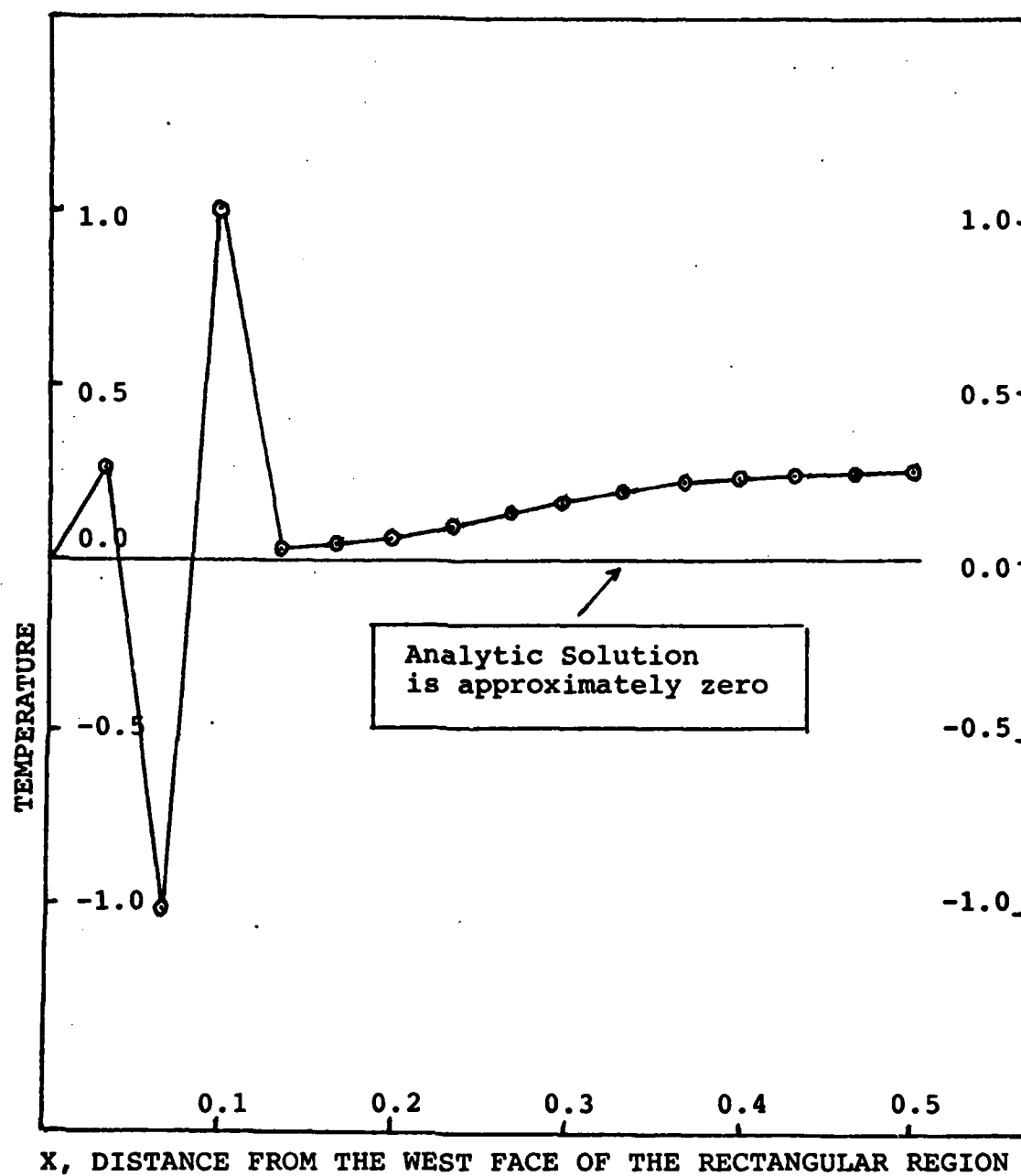


Figure 18. Unstable Oscillations for the Peaceman-Rachford ADI FDMTH for a 31 by 31 Nodal Array. Elapsed Time is 6. Time Step is 1. Number of Iterations is 6. $\kappa = 900$.

Discretization Error.

The Crank-Nicholson implicit FDMTH has the smallest discretization error for large numbers of time steps. The fully explicit FDMTH is the next most accurate FDMTH for large numbers of time steps. The fully implicit FDMTH has a positive discretization error for large numbers of time steps that is larger than the discretization error for the Crank-Nicholson implicit FDMTH. For a sufficiently small time step, the discretization errors of the fully explicit and fully implicit FDMTHs are nearly equal. For large numbers of time steps, the Peaceman-Rachford ADI FDMTH is the least accurate of the FDMTHs studied. The Peaceman-Rachford ADI FDMTH has a negative discretization error that not significantly improved by either decrease in time step size or increase in nodal density. Figure 20 is a comparison of all FDMTHs studied for a time step size of 0.0025 and an elapsed time of 1.

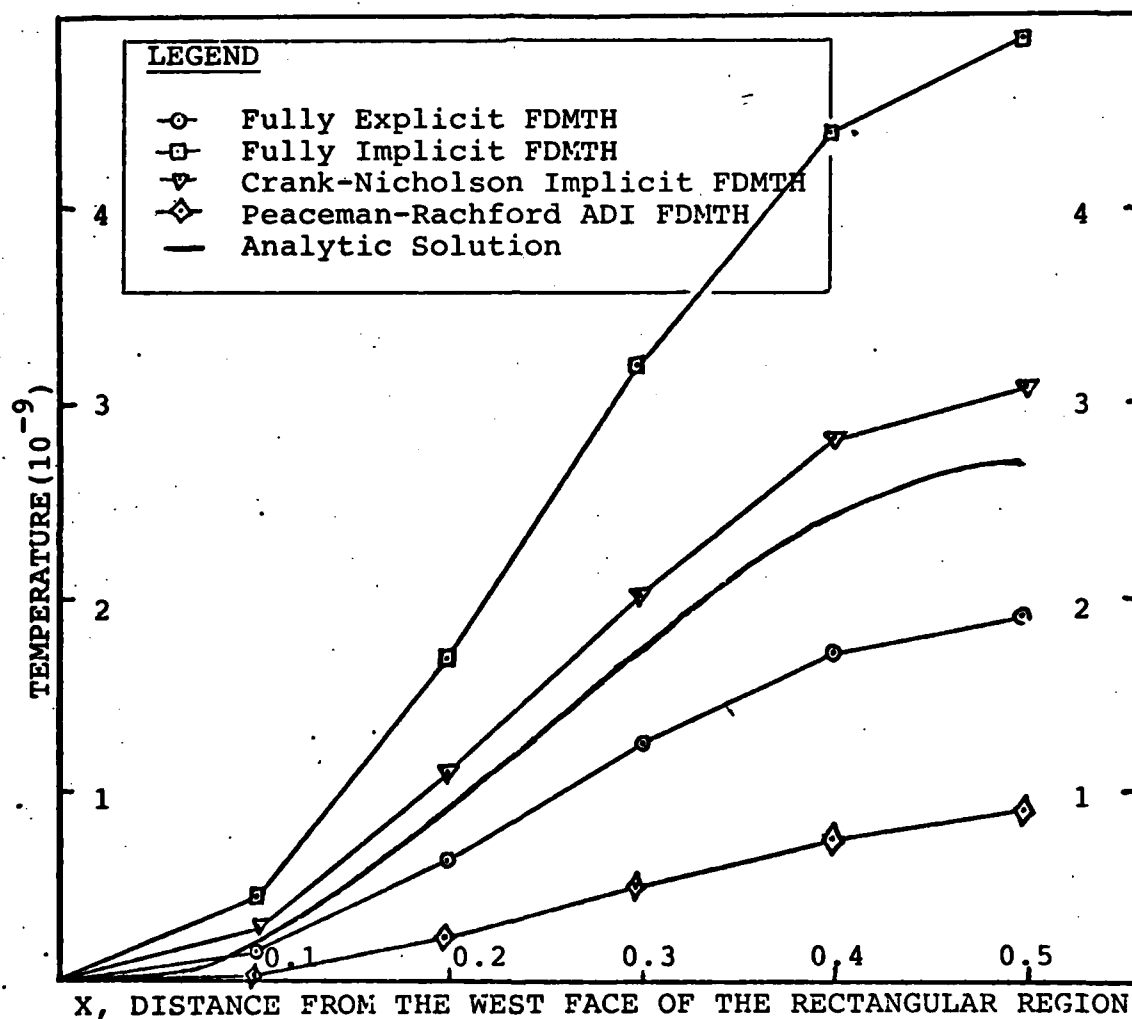


Figure 20. Comparison of FDMTHs for a 11 by 11 Nodal Array. Elapsed Time is 1. Time Step is 0.0025. Number of Iterations is 400. $\kappa = 0.5$ for the Fully Explicit FDMTH. $\kappa = 0.25$ for the Crank-Nicholson and Peaceman-Rachford ADI FDMTHs.

Execution Time.

Data on the execution times of the different FDMTHs was not collected. In general, the fully implicit and Crank-Nicholson implicit FDMTHs were slower because of the use of the Guass-Sidel method of solution. Figures 21 and 22 depict the number of Guass-Sidel iterations required for the fully implicit and Crank-Nicholson implicit FDMTHs, respectively, for a 11 by 11 nodal array and differing size and number of time steps.

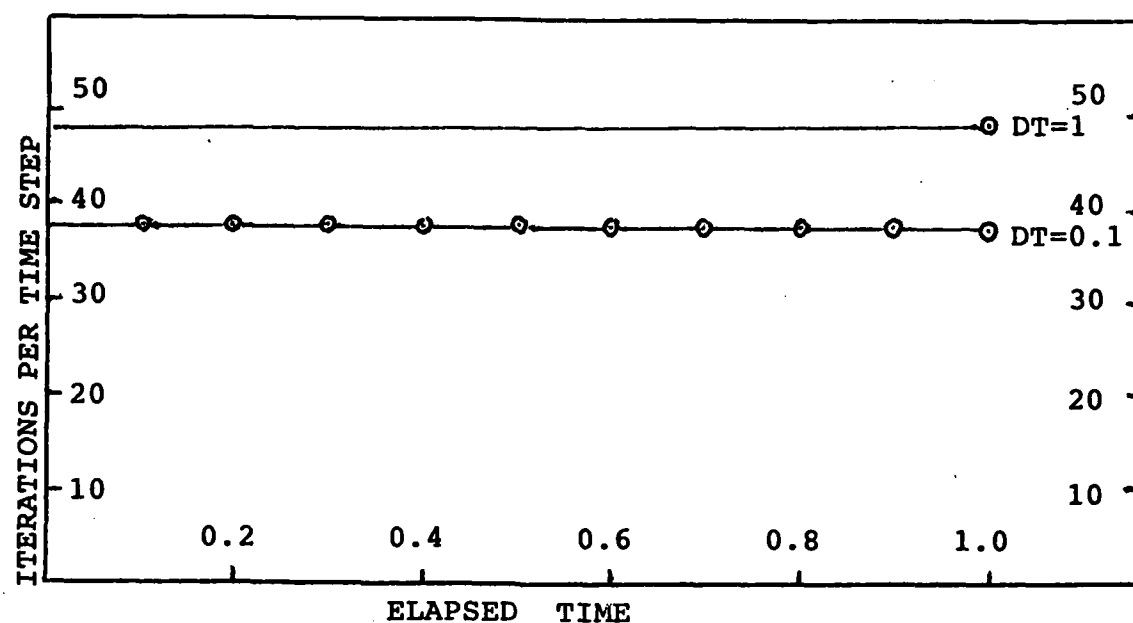


Figure 21. Number of Gauss-Sidel Iterations Required per Time Step for the Fully Implicit FDMTH for a 11 by 11 Nodal Array.

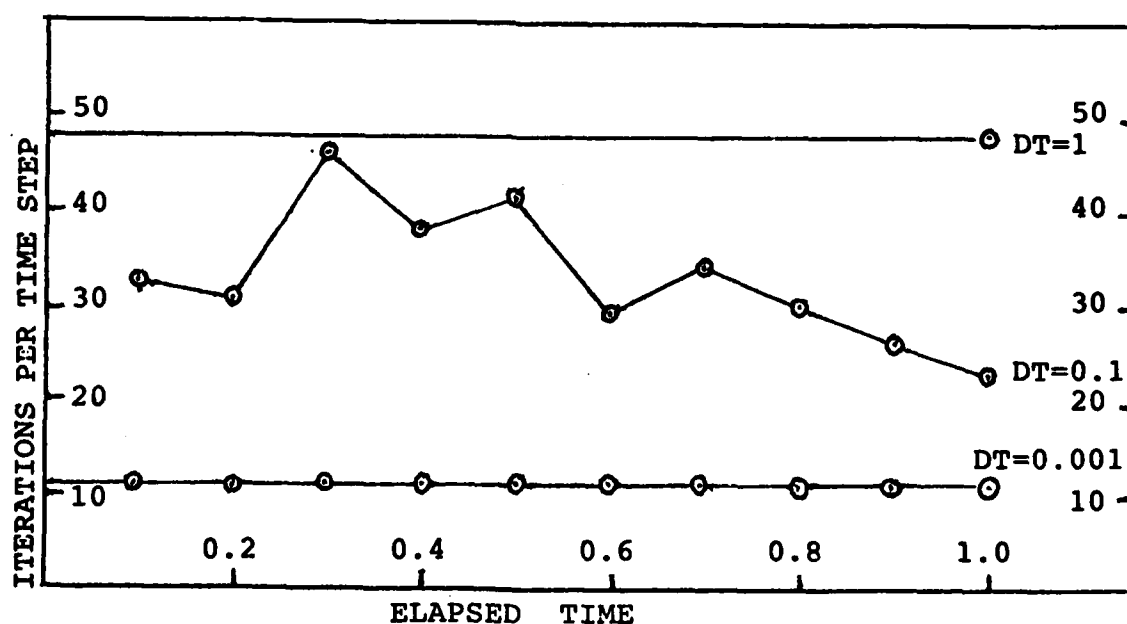


Figure 22. Number of Gauss-Sidel Iterations Required per Time Step for the Crank-Nicholson Implicit FDMTH for a 11 by 11 Nodal Array.

VII. Discussion

All FDMTHs considered gave unrealistic results for a time step of 1 when the maximum initial temperature, TINIT in programs EXPLI, IMPLI, and PRADI; α , the thermal diffusivity; and the dimensions of the rectangular region were equal to 1. The order of the truncation error for all FDMTHs, per Table 2, is also 1 when the size of the time step is 1. The observed unrealistic results for a time step of 1 are probably due to discretization error rather than the type of numerical instability addressed by the stability condition.

The accuracy of all FDMTHs improved with decrease in the size of the time step and/or increase in nodal density. The accuracy of FDMTHs, relative to each other, remained as suggested by the order of the truncation error as long as the size of the time step was small enough for the FDMTHs considered to remain stable. The Peaceman-Rachford ADI FDMTH was the least accurate of the four FDMTHs considered for large numbers of time steps when compared to stable FDMTHs using a common size of time step and nodal array size.

Figures 21 and 22 suggest that the fully implicit and Crank-Nicholson implicit FDMTHs require fewer Gauss-Sidel iterations per time step for smaller time step sizes.

VIII. Conclusions

Stability.

The general stability condition correctly predicts the onset of instability for the fully explicit FDMTH. The fully implicit FDMTH is always stable, as expected. The Crank-Nicholson implicit and Peaceman-Rachford ADI FDMTHs, expected to be unconditionally stable, are unstable for large time step sizes for the initial-boundary value problem studied.

Accuracy.

For sizes of time step satisfying the general stability condition for all four of the FDMTHs considered for large numbers of time steps, the Crank-Nicholson implicit FDMTH is the most accurate FDMTH and the Peaceman-Rachford ADI FDMTH the least accurate for the initial-boundary value problem studied.

Complexity.

The simplest FDMTH algorithm was that of the fully explicit FDMTH.

Stability Condition.

Derivation of the general stability condition by either the matrix method, coefficient method, or proba-

bilistic method leads to the same result,

$$\kappa \equiv \alpha \Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \leq \frac{1}{2} \quad (34)$$

Further, while a FDMTH may be stable when the general stability condition predicts instability, the accuracy of a FDMTH, such as the Peaceman-Rachford ADI FDMTH, is significantly improved if the size of the time step is one for which the general stability condition predicts stability.

IX. Recommendations

Use of This Thesis.

This thesis should be used as a reference or starting point for future studies of FDMTHs to encourage the study of three-dimensional FDMTHs and FDMTH modelling of nuclear effects.

Follow-on Studies.

A follow-on study is needed to better define the regions of stability for two-dimensional FDMTHs, possibly in a manner similar to Table 3 and Figure 12 of this study.

Another study should consider FDMTH solution of a different initial-boundary value problem having a damped analytic solution.

The use of graded spatial grids should be considered as a method of reducing edge effects.

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APPENDIX A

Analytic Solution of the Initial-Boundary Value Problem for Two-Dimensional Transient Heat Conduction(Diffusion)

An initial-boundary value problem describing two-dimensional transient heat conduction(diffusion) for a rectangular region is

$$\frac{\partial T}{\partial t} = \alpha \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] \quad (\text{A-1a})$$

$$T(0,y,t) = T(a,y,t) = T(x,0,t) = T(x,b,t) = 0 \quad (\text{A-1b})$$

$$T(x,y,0) = \sin \pi x \sin \pi y \quad (\text{A-1c})$$

where T is for temperature, α is the thermal diffusivity, x and y are spatial dimensions, and t is for time.

The solution for $T(x,y)$ follows.

Let $T(x,y,t) = F(x,y)G(t)$,

then $\partial T / \partial t \equiv T_t = FG_t$, $\partial^2 T / \partial x^2 \equiv T_{xx} = F_{xx}G$,

and $\partial^2 T / \partial y^2 \equiv T_{yy} = F_{yy}G$.

Now, $FG_t = \alpha [F_{xx}G + F_{yy}G]$,

or $G_t / G = \lambda = \alpha [F_{xx} / F + F_{yy} / F]$.

Let $F(x,y) = H(x)Q(y)$, then $F_{xx} = H_{xx}Q$, and $F_{yy} = HQ_{yy}$.

$$\lambda = \alpha[H_{xx}Q/HQ + HQ_{yy}/HQ] = \alpha[H_{xx}/H + Q_{yy}/Q]$$

$$\lambda/\alpha = H_{xx}/H + Q_{yy}/Q$$

$$H_{xx}/H = \xi = \lambda/\alpha - Q_{yy}/Q$$

Solve $H_{xx}/H = \xi$ for H .

$$[D^2 - \xi]H = 0 \quad H = \hat{c}_1 \sinh \sqrt{-\xi x} = \hat{c}_2 \cosh \sqrt{-\xi x}.$$

Applying the boundary condition $H(0) = 0$,

$$0 = \hat{c}_2 \cosh 0 \rightarrow \hat{c}_2 = 0, \text{ or } H = \hat{c}_1 \sinh \sqrt{-\xi x},$$

$$\text{or } H = \tilde{c}_1 \sin \sqrt{\xi x} \text{ (by the trigonometric identity: } \sinh \sqrt{-1} u = \sin \sqrt{u} \text{)}.$$

Applying the boundary condition $H(a) = 0$,

$$0 = \tilde{c}_1 \sin \sqrt{\xi a} \rightarrow m\pi = a\sqrt{\xi} \rightarrow \xi = m^2 \pi^2 / a^2, m=0,1,2, \dots$$

or

$$H = \tilde{c}_1 \sin[m\pi x/a].$$

Similarly, $Q = \tilde{d}_1 \sin[n\pi y/b]$,

$$\text{or } F = \tilde{c}_1 \tilde{d}_1 \sin[m\pi x/a] \sin[n\pi y/b].$$

When solving for Q, it is also found that

$$n\pi = \sqrt{\lambda/\alpha} - \xi b \rightarrow n^2\pi^2/b^2 = \lambda/\alpha - \xi,$$

$$\text{or } \lambda = \alpha(n^2\pi^2/b^2 + \xi) = \alpha(n^2\pi^2/b^2 + m^2\pi^2/a^2).$$

Solving $G_t/G = \lambda$, for G,

$$[D - \lambda]G = 0 \rightarrow G = f \exp[\alpha(m^2\pi^2/a^2 + n^2\pi^2/b^2)t]$$

or,

$$T(x,y,t) = C \exp[-\alpha(m^2\pi^2/a^2 + n^2\pi^2/b^2)t] \sin[m\pi x/a] \sin[n\pi y/b].$$

APPENDIX B

Matrix Method Derivation of the Stability Condition for the Two-Dimensional Finite Difference Approximation of Transient Heat Conduction(Diffusion)

The general two-dimensional finite difference approximation of transient heat conduction(diffusion) is

$$\begin{aligned}
 T_P^{k+1} - T_P^k &= \frac{\alpha \Delta t}{(\Delta x)^2} [f_E T_E^{k+1} + (1-f_E) T_E^k \\
 &\quad + f_W T_W^{k+1} + (1-f_W) T_W^k \\
 &\quad - 2f_{P_{EW}} T_P^{k+1} - 2(1-f_{P_{EW}}) T_P^k] \\
 &\quad + \frac{\alpha \Delta t}{(\Delta y)^2} [f_N T_N^{k+1} + (1-f_N) T_N^k \\
 &\quad + f_S T_S^{k+1} + (1-f_S) T_S^k \\
 &\quad - 2f_{P_{NS}} T_P^{k+1} - 2(1-f_{P_{NS}}) T_P^k] \quad (B-1)
 \end{aligned}$$

or

$$\begin{aligned} aT_P^{k+1} - bT_E^{k+1} - bT_W^{k+1} - cT_N^{k+1} - cT_S^{k+1} \\ = a'T_P^k + b'T_E^k + b'T_W^k + c'T_N^k + c'T_S^k \end{aligned} \quad (B-2)$$

where

$$a = 1 + \frac{2\alpha\Delta t f_x}{(\Delta x)^2} + \frac{2\alpha\Delta t f_y}{(\Delta y)^2}$$

$$a' = 1 - \frac{2\alpha\Delta t (1-f_x)}{(\Delta x)^2} - \frac{2\alpha\Delta t (1-f_y)}{(\Delta y)^2}$$

$$\begin{aligned} b &= \alpha\Delta t f_x / (\Delta x)^2 \\ b' &= \alpha\Delta t (1-f_x) / (\Delta x)^2 \\ c &= \alpha\Delta t f_y / (\Delta y)^2 \\ c' &= \alpha\Delta t (1-f_y) / (\Delta y)^2 \end{aligned}$$

and

$$f_x = f_E = f_W = f_{P_{EW}}$$

and

$$f_y = f_N = f_S = f_{P_{NS}}$$

The matrix equivalent to equation (B-2) is

$$\underline{A} \underline{T}^{k+1} = \underline{A'} \underline{T}^k. \quad (B-3)$$

or as depicted on the next page.

$$\begin{pmatrix}
 a & -b & \dots & -c \\
 -b & a & -b & \dots & -c \\
 \cdot & -b & a & -b & \dots & -c \\
 \vdots & & & & & \cdot \\
 -c & & & & & -c \\
 & & & & & \vdots \\
 & & & & & \vdots \\
 & & & & -b & a & -b \\
 & & -c & \dots & -b & a
 \end{pmatrix}
 \begin{pmatrix}
 T_1^{k+1} \\
 T_2^{k+1} \\
 T_3^{k+1} \\
 \vdots \\
 \vdots \\
 \vdots \\
 T_{mdl}^{k+1}
 \end{pmatrix}$$

$$=
 \begin{pmatrix}
 a' & -b' & \dots & -c' \\
 -b' & a' & -b' & \dots & -c' \\
 \cdot & -b' & a' & -b' & \dots & -c' \\
 \vdots & & & & & \cdot \\
 -c' & & & & & -c' \\
 & & & & & \vdots \\
 & & & & & \vdots \\
 & & & & -b' & a' & -b' \\
 & & -c' & & -b' & a'
 \end{pmatrix}
 \begin{pmatrix}
 T_1^k \\
 T_2^k \\
 T_3^k \\
 \vdots \\
 \vdots \\
 \vdots \\
 T_{mdl}^k
 \end{pmatrix}
 \tag{B-4}$$

The eigenvalues of A' are equal to the eigenvalues of $[\underline{I} - (\underline{A}' - \underline{I})]$. $(\underline{A}' - \underline{I})$ is the coefficient matrix of the finite difference representation of the boundary value problem

$$\lambda_s T = T_{xx} + T_{yy} \quad (B-5)$$

$$T(0,y) = T(1,y) = T(x,0) = T(x,1) = 0$$

Solving for T,

$$T(x,y) = F(x)G(y)$$

$$T_{xx} = F_{xx}G$$

$$T_{yy} = FG_{yy}$$

$$\text{or } \lambda_s FG = F_{xx}G + FG_{yy} \rightarrow \lambda_s - F_{xx}/F = G_{yy}/G$$

$$\frac{-F_{xx}}{F} + \lambda_s = \xi = \frac{G_{yy}}{G}$$

$$-F_{xx} + (\lambda_s - \xi)F = 0$$

$$[D^2 + (\xi - \lambda_s)]F = 0, \text{ let } \eta = \xi - \lambda_s$$

$$F = \hat{c}_1 \sinh \sqrt{-\eta x} + \hat{c}_2 \sinh \sqrt{-\eta x}$$

$$F(0) = 0 = \hat{c}_2 \cosh 0 \rightarrow \hat{c}_2 = 0$$

$$F = \hat{c}_1 \sinh \sqrt{-\eta x}$$

$$F(1) = 0 = \hat{c}_1 \sin \sqrt{\eta} \rightarrow \sqrt{\eta} = s\pi$$

$$F = \tilde{c}_1 \sin(s\pi x)$$

for $G_{yy} - \xi G = 0$, as for F ,

$$G = \bar{d}_1 \sin(t\pi y)$$

$$\text{and } T = C \sin(s\pi x) \sin(t\pi y) .$$

$$\text{Let } T = \sin(s\pi x) \sin(t\pi y) .$$

A finite difference representation of equation (B-1)
is

$$\begin{aligned} & b'T(i+1,j) - 2b'T(i,j) + b'T(i-1,j) \\ & + c'T(i,j+1) - 2c'T(i,j) + c'T(i,j-1) = \lambda_s T(i,j) \end{aligned} \quad (B-6)$$

or as shown on the next page.

$$b' \sin\left[\frac{m\pi si}{M} + \frac{m\pi s}{M}\right] \sin\left[\frac{n\pi tj}{N}\right]$$

$$- 2b' \sin\left[\frac{m\pi si}{M}\right] \sin\left[\frac{n\pi tj}{N}\right]$$

$$+ b' \sin\left[\frac{m\pi si}{M} - \frac{m\pi s}{M}\right] \sin\left[\frac{n\pi tj}{N}\right]$$

$$c' \sin\left[\frac{m\pi si}{M}\right] \sin\left[\frac{n\pi tj}{N} + \frac{n\pi t}{N}\right]$$

$$- 2c' \sin\left[\frac{m\pi si}{M}\right] \sin\left[\frac{n\pi tj}{N}\right]$$

$$+ c' \sin\left[\frac{m\pi si}{M}\right] \sin\left[\frac{n\pi tj}{N} - \frac{n\pi t}{N}\right]$$

$$= \lambda_s \sin\left[\frac{m\pi si}{M}\right] \sin\left[\frac{n\pi tj}{N}\right] \quad (B-7)$$

Using the trigonometric identity,

$$\sin\alpha\cos\beta = \frac{1}{2}\sin(\alpha+\beta) + \frac{1}{2}\sin(\alpha-\beta) ,$$

and dividing through by $\sin(m\pi s/M)\sin(n\pi t/N)$, equation (B-7) reduces to

$$2b'\cos[m\pi s/M] - 2b' + 2c'\cos[n\pi t/N] - 2c' = \lambda_s \quad (B-8)$$

By the trigonometric identity,

$$\sin^2\alpha = \frac{1}{2}(1-\cos 2\alpha) ,$$

equation (B-8) reduces to

$$\lambda_s = -4[b'\sin^2(m\pi s/2M) + c'\sin^2(n\pi t/2N)] \quad (B-9)$$

For equation (B-9) to be stable, must have that

$$1 \leq | 1 - 4[b'\sin^2(m\pi s/2M) + c'\sin^2(n\pi t/2N)] | \quad (B-10)$$

or

$$-1 \leq 1 - 4[b'\sin^2(m\pi s/2M) + c'\sin^2(n\pi t/2N)] \quad (B-11)$$

or, since $\sin^2\alpha \leq 1$,

$$\frac{1}{4} \geq b' + c' . \quad (B-12)$$

Or, the general stability condition is

$$\kappa \equiv \alpha\Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \leq \frac{1}{4} \quad (B-13)$$

APPENDIX C

Coefficient Method Derivation of the Stability Condition for the Two-Dimensional Finite Difference Approximation of Transient Heat Conduction(Diffusion)

The general two-dimensional finite difference approximation of transient heat conduction(diffusion) is as given in Appendix B, equation (B-1), or

$$\begin{aligned} (1+2p+2q)T_P^{k+1} - pT_E^{k+1} - pT_W^{k+1} - qT_N^{k+1} - qT_S^{k+1} \\ = (1-2p'-2q')T_P^k + p'T_E^k + p'T_W^k + q'T_N^k + q'T_S^k \end{aligned} \quad (C-1)$$

$$\begin{aligned} \text{where } p &= \alpha \Delta t f_x / (\Delta x)^2 \\ q &= \alpha \Delta t f_y / (\Delta y)^2 \\ p' &= \alpha \Delta t (1-f_x) / (\Delta x)^2 \\ q' &= \alpha \Delta t (1-f_y) / (\Delta y)^2 \\ f_x &= f_E = f_W = f_{P_{EW}} \end{aligned}$$

$$\text{and } f_y = f_N = f_S = f_{P_{NS}} .$$

The ratio of T_P^{k+1} to T_P^k , λ , from equation (C-1) is

$$\begin{aligned} \lambda = \frac{(1-2p'-2q')}{(1+2p+2q)} + \frac{p(T_E^{k+1} + T_W^{k+1}) + q(T_N^{k+1} + T_S^{k+1})}{(1+2p+2q)} \\ + \frac{p'(T_E^k + T_W^k) + q'(T_N^k + T_S^k)}{(1+2p+2q)} \end{aligned} \quad (C-2)$$

Both Myers and Patankar consider only the case of a single interior node so that $T_E = T_W = T_N = T_S = 0$. For a single interior node,

$$\lambda = \frac{1-2p'-2q'}{1+2p+2q} \quad (C-3)$$

The stability curves predicted by (C-3) are depicted in Figure C-1. The general stability condition can be derived from equation (C-3) as follows:

$$\lambda = \frac{1 - 2\alpha\Delta t(1-f_x)/(\Delta x)^2 - 2\alpha\Delta t(1-f_y)/(\Delta y)^2}{1 - 2\alpha\Delta t f_x/(\Delta x)^2 + 2\alpha\Delta t f_y/(\Delta y)^2} \quad (C-4)$$

For stability, λ must be positive. The denominator of equation (C-6) is always positive, so only the numerator need be considered further. For stability then

$$0 \leq 1 - 2\alpha\Delta t(1-f_x)/(\Delta x)^2 - 2\alpha\Delta t(1-f_y)/(\Delta y)^2$$

or

$$\frac{1}{2} \geq \alpha\Delta t[(1-f_x)/(\Delta x)^2 + (1-f_y)/(\Delta y)^2] .$$

Or, the general stability condition is

$$\kappa \equiv \alpha\Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \leq \frac{1}{2} . \quad (C-5)$$

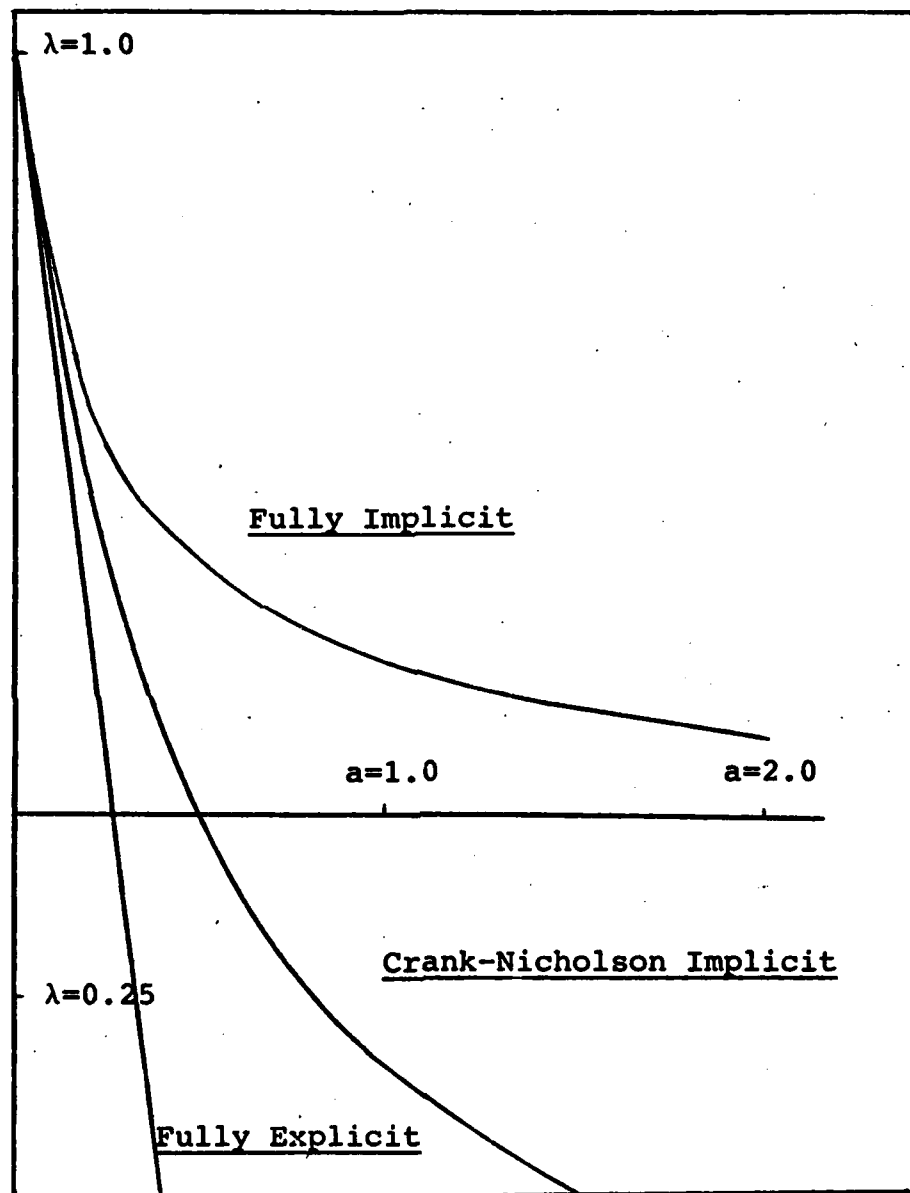


Figure C-1. Finite Difference Stability Curves for Transient Heat Conduction (Diffusion) in a Square Region with One Interior Node

$$a = \frac{\alpha \Delta t}{(\Delta x)^2}$$

APPENDIX D

Probabilistic Method Derivation of the Stability Condition for the Two-Dimensional Finite Difference Approximation of Transient Heat Conduction(Diffusion)

The general two-dimensional finite difference approximation of transient heat conduction(diffusion) is as given in Appendix B, equation (B-1). Let P_e^{k+1} be the probability of node P attaining the potential(temperature) of node e at time $t \pm i\Delta t$, then

$$P_P^{k+1} = 1 \quad (D-1)$$

$$P_E^{k+1} = \alpha \Delta t f_E / (W) (\Delta x)^2 \quad (D-2)$$

$$P_W^{k+1} = \alpha \Delta t f_W / (W) (\Delta x)^2 \quad (D-3)$$

$$P_N^{k+1} = \alpha \Delta t f_N / (W) (\Delta y)^2 \quad (D-4)$$

$$P_S^{k+1} = \alpha \Delta t f_S / (W) (\Delta y)^2 \quad (D-5)$$

$$P_P^k = \frac{[1 - 2\alpha \Delta t (1-f_{P_{EW}}) / (\Delta x)^2 - 2\alpha \Delta t (1-f_{P_{NS}}) / (\Delta y)^2]}{W} \quad (D-6)$$

$$P_E^k = \alpha \Delta t (1-f_E) / (W) (\Delta x)^2 \quad (D-7)$$

$$P_W^k = \alpha \Delta t (1-f_W) / (W) (\Delta x)^2 \quad (D-8)$$

$$P_N^k = \alpha \Delta t (1-f_N) / (W) (\Delta y)^2 \quad (D-9)$$

$$P_S^k = \alpha \Delta t (1-f_S) / (W) (\Delta y)^2 \quad (D-10)$$

$$\text{and } W = 1 + \alpha \Delta t f_{P_{EW}} / (\Delta x)^2 + \alpha \Delta t f_{P_{NS}} / (\Delta y)^2 . \quad (D-11)$$

Using the probabilistic coefficients defined on the previous page, the general FDMTH becomes

$$\begin{aligned} P_P^{k+1} T_P^{k+1} &= P_E^{k+1} T_E^{k+1} + P_W^{k+1} T_W^{k+1} + P_N^{k+1} T_N^{k+1} + P_S^{k+1} T_S^{k+1} \\ &+ P_E^k T_E^k + P_W^k T_W^k + P_N^k T_N^k + P_S^k T_S^k + P_P^k T_P^k . \end{aligned} \quad (D-12)$$

As long as all f_e are less than or equal to 1, the only probabilistic coefficient that might be negative is P_P^k . Since negative probabilities are not realistic, the following stability condition is inferred.

$$1 - 2\alpha \Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \geq 0 \quad (D-13)$$

or

$$\kappa \equiv \alpha \Delta t \left[\frac{(1-f_x)}{(\Delta x)^2} + \frac{(1-f_y)}{(\Delta y)^2} \right] \leq \frac{1}{2} , \quad (D-14)$$

where

$$f_x = f_E = f_W = f_{P_{EW}}$$

$$f_y = f_N = f_S = f_{P_{NS}} .$$

Equation (D-14) is the general stability condition for the two-dimensional finite difference approximation of transient heat conduction(diffusion).

APPENDIX E

FDMTH Data

The volume of data generated in this study was too great to graphically portray all of it. The data presented in this appendix represents most of the more significant data collected and not previously described in Section VI, Results.

List of Figures.

<u>Figure</u>	<u>Page</u>
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E-1-2	Unstable Oscillations for the Peaceman-Rachford ADI FDMTH for a 31 by 31 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 20. Time Step is 1. Number of Iterations is 20.
E-2-1	Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 6. Time Step is 1. Number of Iterations is 6.
E-2-2	Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.2. Time Step is 0.01. Number of Iterations is 20.
E-2-3	Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 1. Time Step is 0.001. Number of Iterations is 1000.

Figure

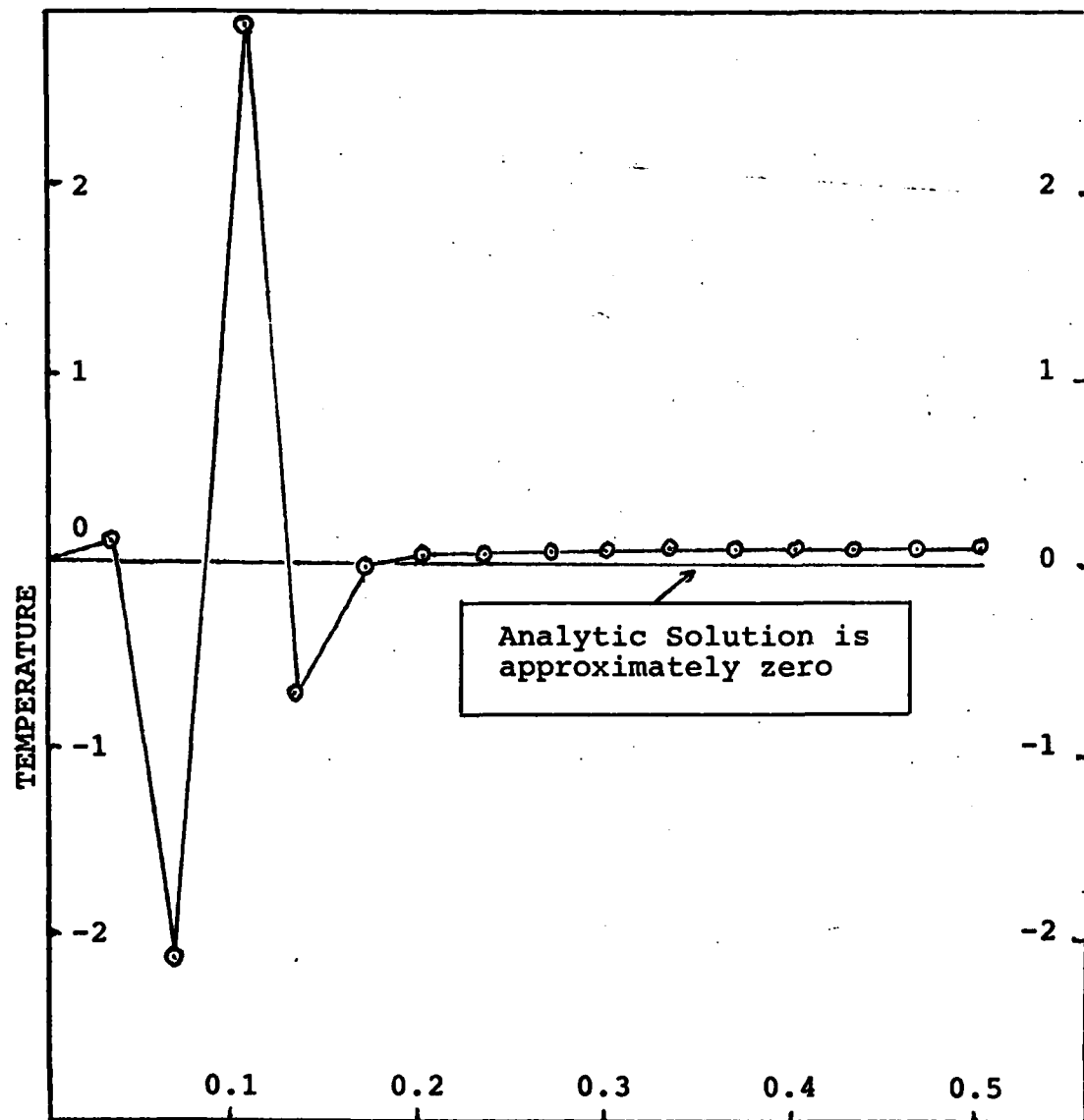
Page

- E-2-4 Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.1. Time Step is 0.0001. Number of Iterations is 1000.
- E-2-5 Comparison of FDMTHs for a 21 by 21 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 2. Time Step is 1. Number of Iterations is 2.
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- E-3-1 Number of Oscillations by Node for the Peaceman-Rachford ADI FDMTH for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.5. Time Step is 0.0001. Number of Iterations is 5000.
- E-3-2 Number of Oscillations by Node for the Crank-Nicholson Implicit FDMTH for a 21 by 21 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.01. Time Step is 0.0001. Number of Iterations is 100.

Acronyms.

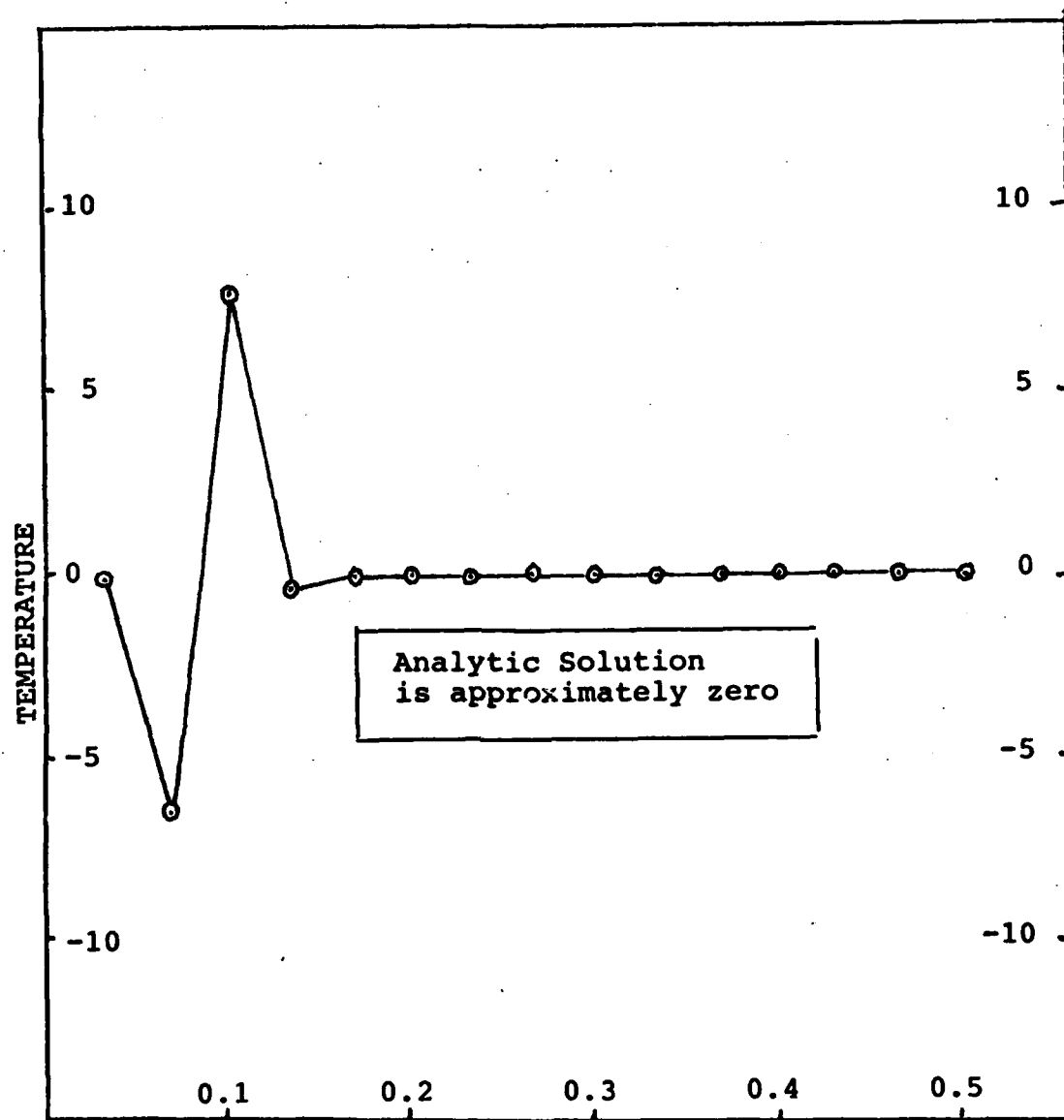
The following acronyms are used in the figures of this appendix.

ANALY	Analytic Solution
EXPLI	Fully Explicit FDMTH
IMPLI	Fully Implicit FDMTH
CNICH	Crank-Nicholson Implicit FDMTH
PRADI	Peaceman-Rachford ADI FDMTH



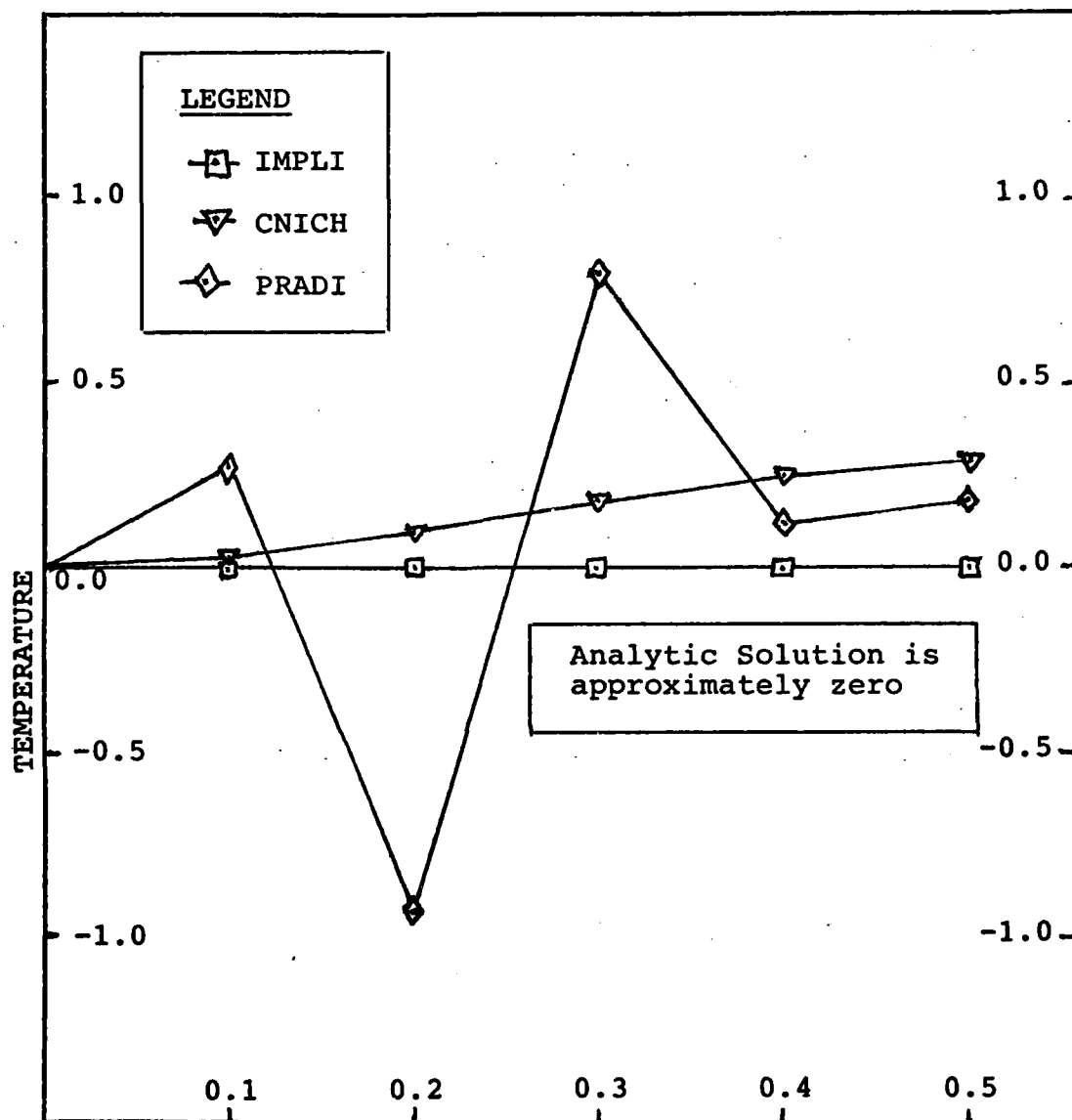
X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure E-1-1. Unstable Oscillations for the Peaceman-Rachford ADI FDMTH for a 31 by 31 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 10. Time Step is 1. Number of Iterations is 10. $\kappa = 900$.



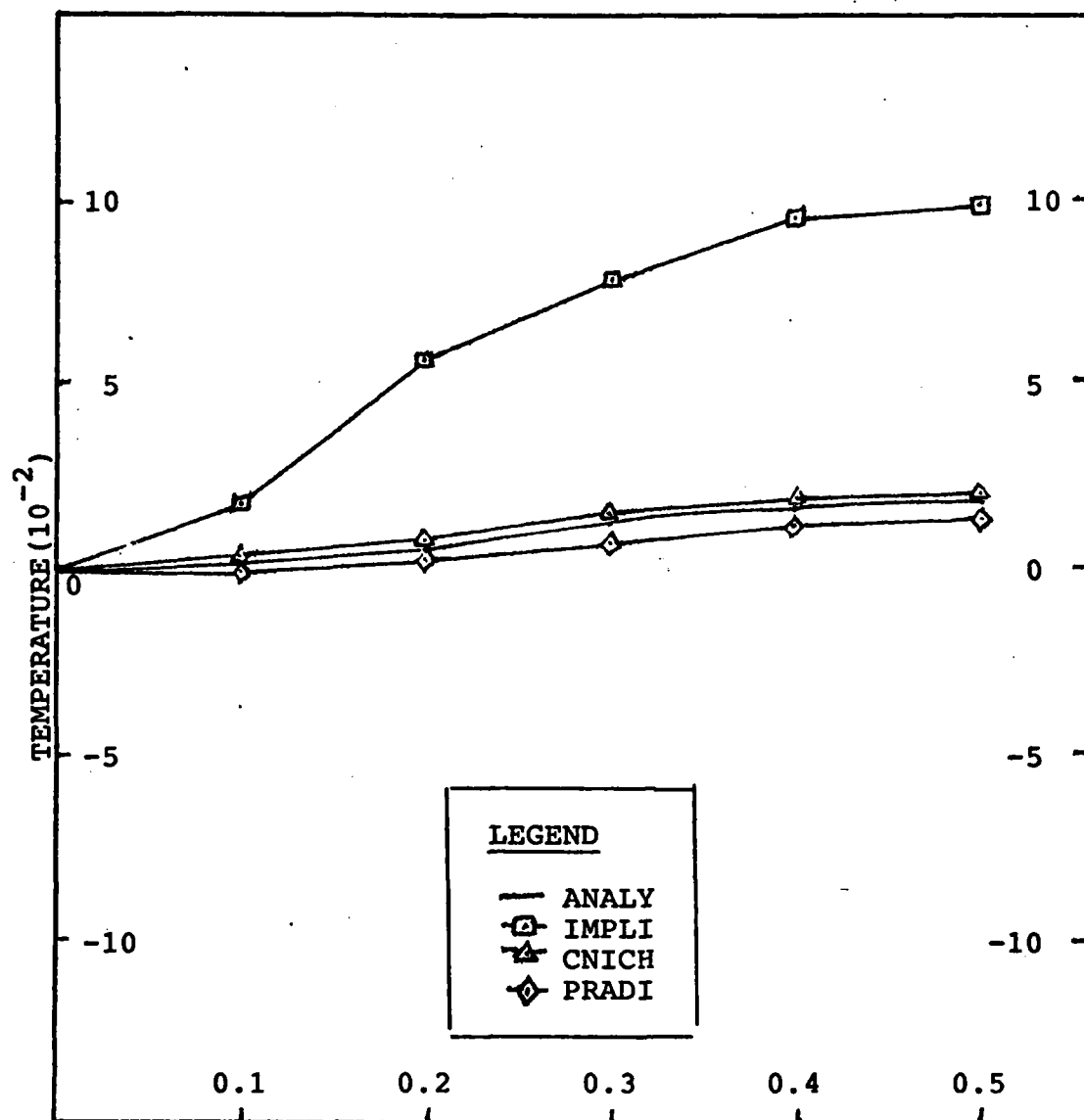
X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure E-1-2. Unstable Oscillations for the Peaceman-Rachford ADI FDMTH for a 31 by 31 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 20. Time Step is 1. Number of Iterations is 20.
 $\kappa = 900$.



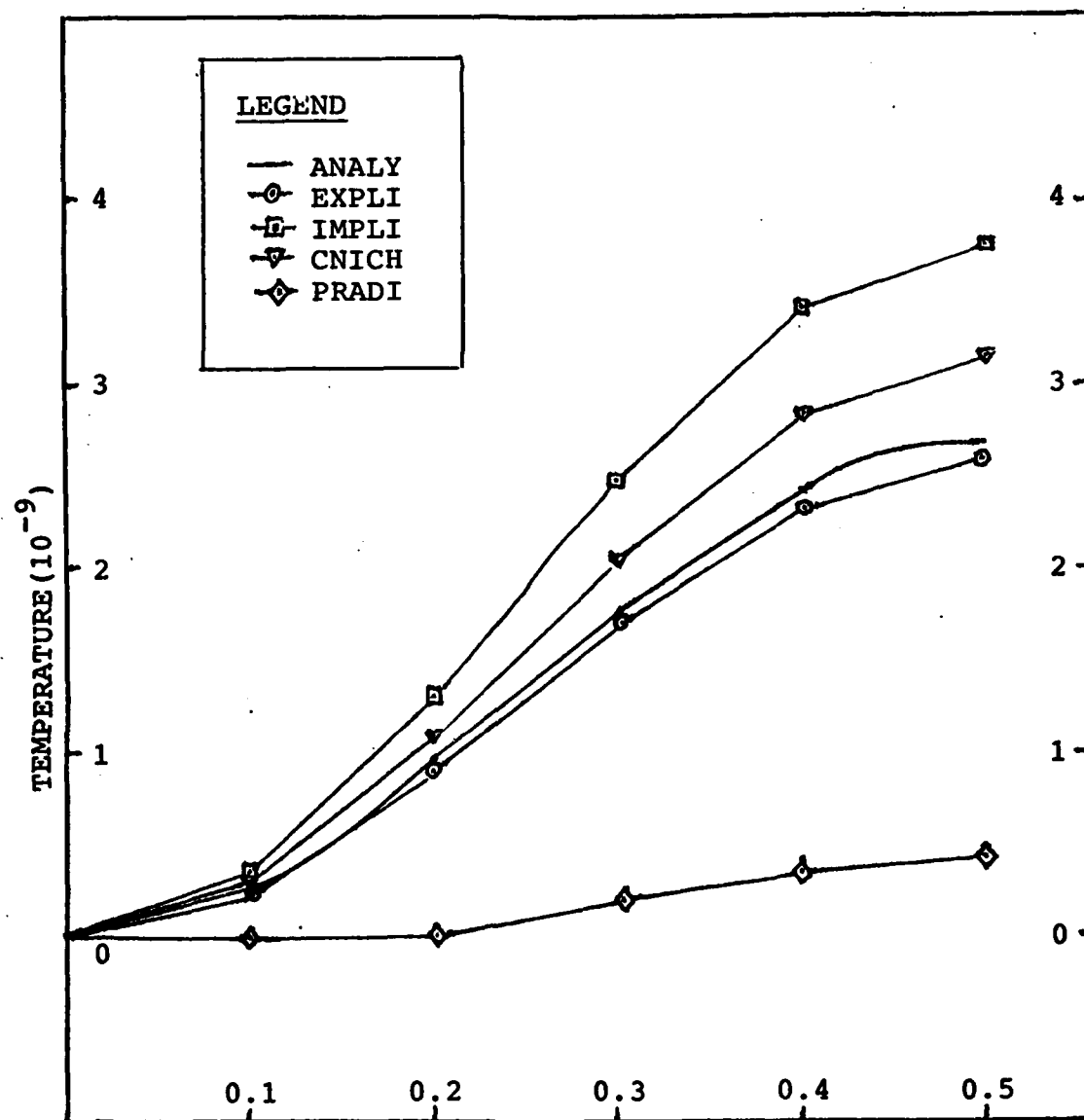
X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure E-2-1. Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 6. Time Step is 1. Number of Iterations is 6.



X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure E-2-2. Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.2. Time Step is 0.01. Number of Iterations is 20.



X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure E-2-3. Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 1. Time Step is 0.001. Number of Iterations is 1000.

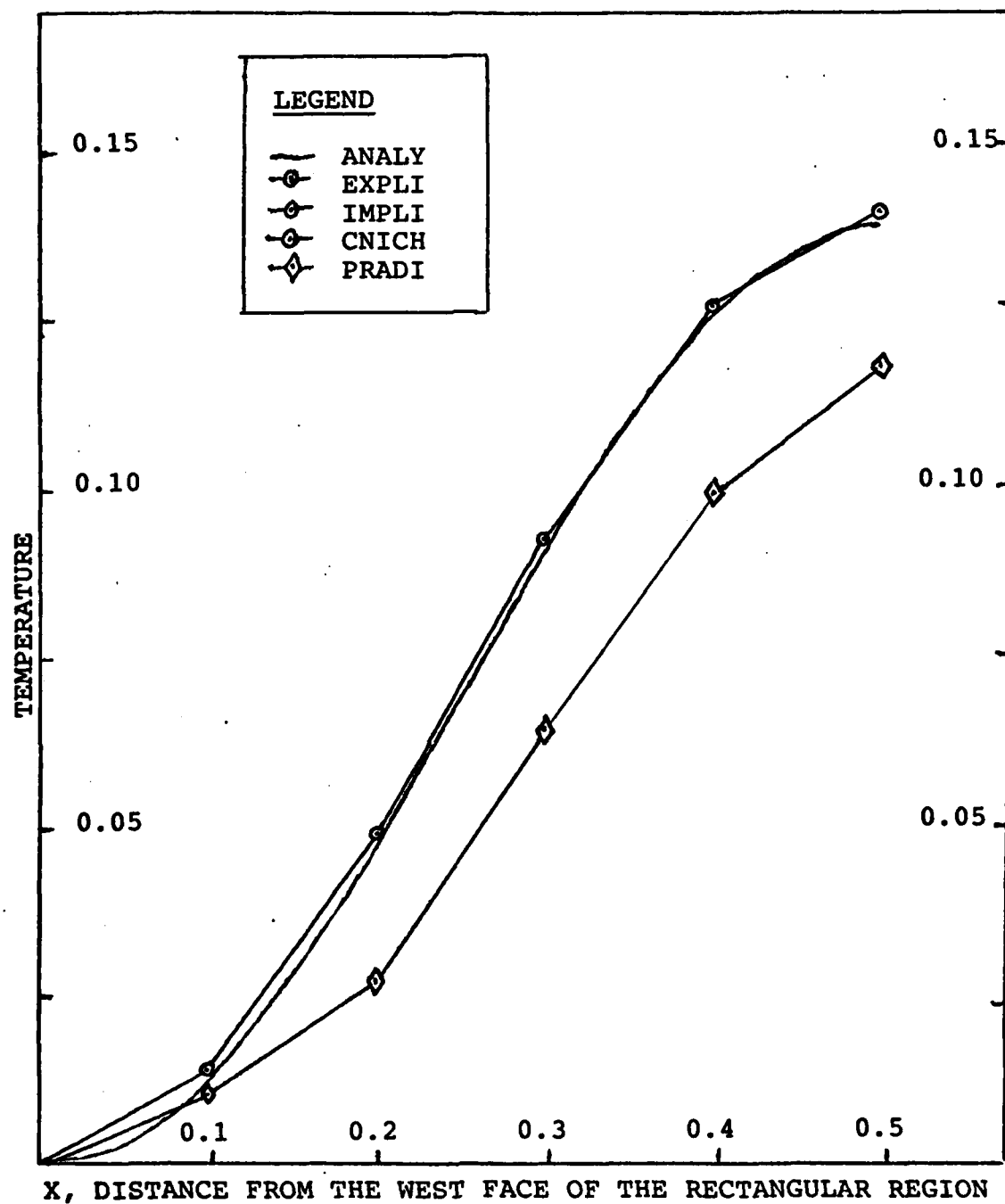


Figure E-2-4. Comparison of FDMTHs for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.1. Time Step is 0.0001. Number of Iterations is 1000.

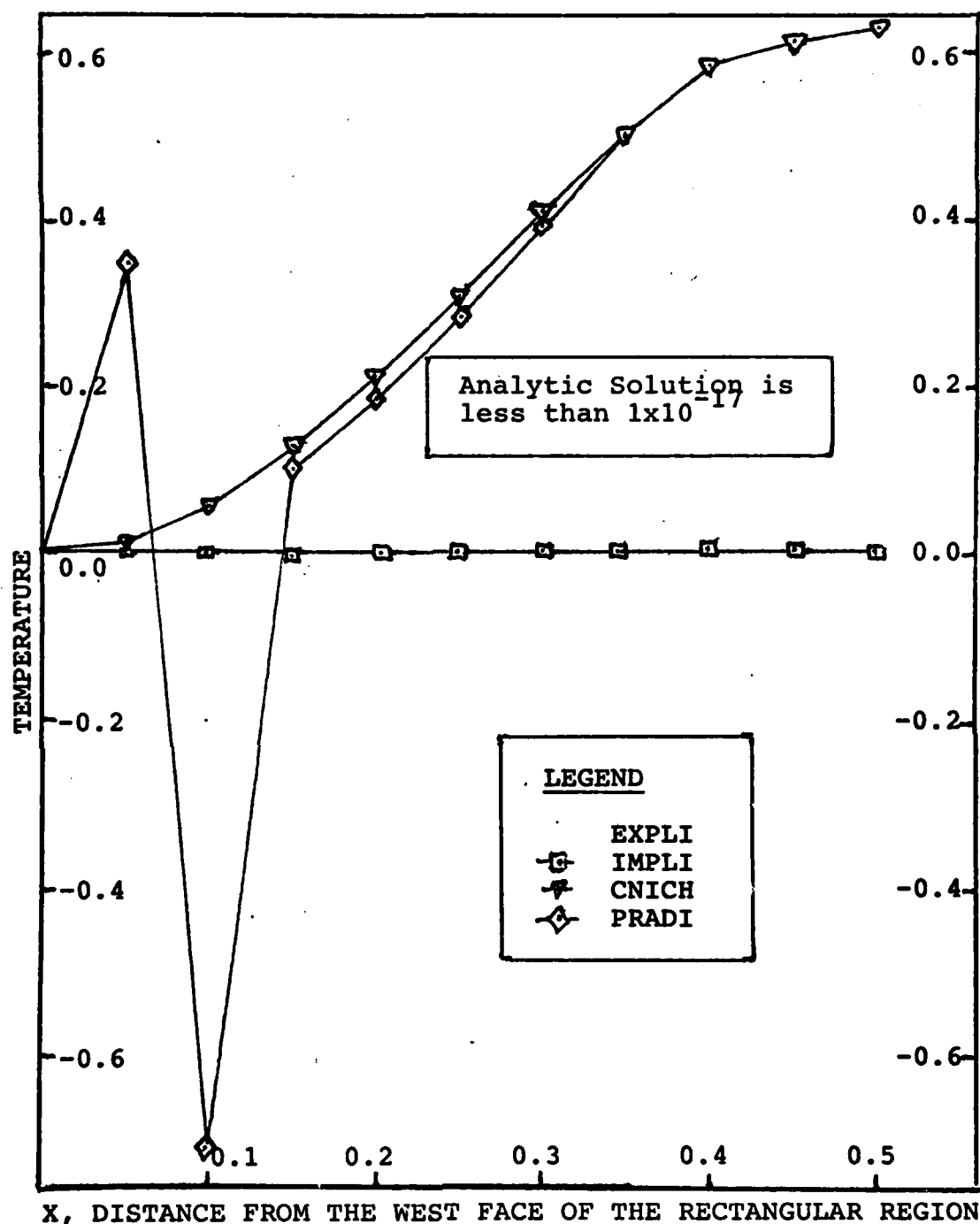
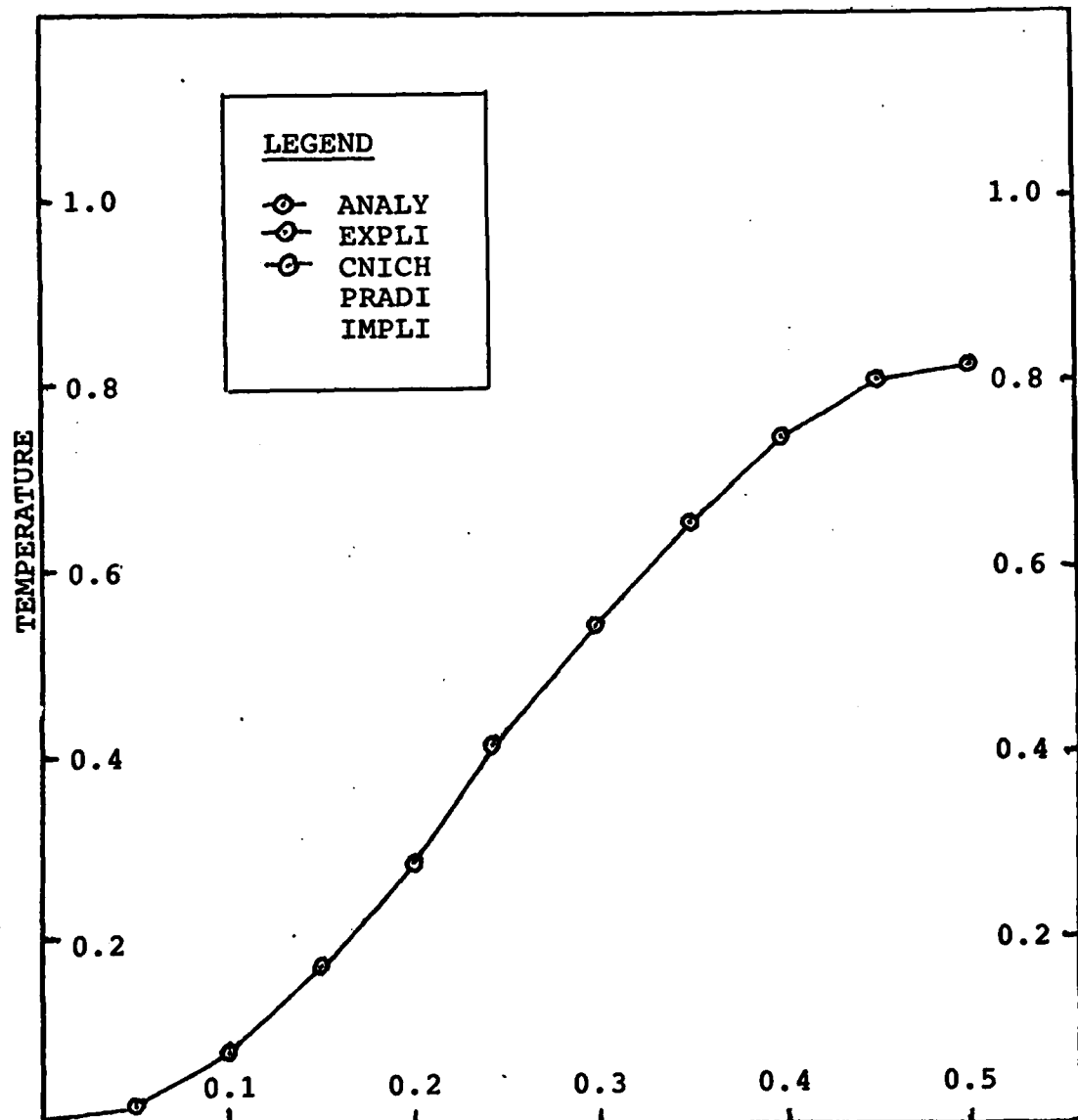


Figure E-2-5. Comparison of FDMTHs for a 21 by 21 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 2. Time Step is 1. Number of Iterations is 2.



X, DISTANCE FROM THE WEST FACE OF THE RECTANGULAR REGION

Figure E-2-6. Comparison of FDMTHs for a 21 by 21 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.01. Time Step is 0.0001. Number of Iterations is 100.

[illegible]

Figure E-3-1. Number of Oscillations by Node for the Peaceman-Rachford ADI FDMTH for a 11 by 11 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.5. Time Step is 0.0001. Number of Iterations is 5000.

[illegible]

Figure E-3-2. Number of Oscillations by Node for the Crank-Nicholson Implicit FDMTH for a 21 by 21 Nodal Array Imposed Over a 1 by 1 Rectangular Region. Elapsed Time is 0.01. Time Step is 0.0001. Number of Iterations is 100.

APPENDIX F

Use of Band Storage to Reduce Computer Program Memory Requirements for Coefficient Matrices¹

This appendix presents, by example, the use made of band storage for storage of banded coefficient matrices characteristic of the fully implicit, Crank-Nicholson implicit, and Peaceman-Rachford alternating direction implicit (ADI) finite difference methods (FDMTHs). For an m by n nodal array imposed over a rectangular region, application of any of the forementioned FDMTHs results in a banded coefficient matrix. For the Peaceman-Rachford ADI FDMTH, the resulting coefficient matrix is tridiagonal. For the fully implicit and Crank-Nicholson implicit FDMTHs, the resulting coefficient matrix has a band width of $2M-1$ or $2N-1$ depending on the order in which the nodes are numbered. $M = m - 1$ and $N = n - 1$. The variables M and N are introduced for a convenience in coefficient subscripting described later. The remainder of this appendix is concerned with the coefficient matrices of the fully implicit and Crank-Nicholson implicit FDMTHs. The coefficient matrix of the Peaceman-Rachford ADI FDMTH may be band stored with minor modifications to the following.

¹Alan Jennings, Matrix Computations for Engineers and Scientists, (London: John Wiley and Sons, Inc., 1977) pp. 95-96.

The coefficient matrix is dimensioned MDL by MDL for the fully implicit and Crank-Nicholson FDMTHs where $MDL = (M-1) \text{ times } (N-1)$. In the nodal array is, for example, 31 by 31, then $M = N = 30$ and the coefficient matrix is 841 by 841. By taking advantage of the banded nature of coefficient matrices for the fully implicit and the Crank-Nicholson FDMTHs; and, noting that, when using the Gauss-Seidel solution technique, no use is made of the zero-valued coefficients not within the banded portion of the coefficient matrix; the coefficient matrix can be represented by a band storage array dimensioned $(2M-1)$ by MDL. For a 31 by 31 nodal array, the band storage array is dimensioned 59 by 841, or less than one tenth of the size of the coefficient matrix that it replaces, dimensioned 841 by 841. The following example illustrates the application of band storage.

Consider the coefficient matrix for the fully implicit FDMTH for a 5 by 5 nodal array, shown in Figure F-1, where coefficients not shown are zero-valued and outside the band of interest. In this case, $M = N = 4$ and the band width is 7. If zeros are added to the band of Figure F-1 so that the band resembles a parallelogram as shown in Figure F-2, then a new coefficient matrix of dimension 7 by 9 can be defined whose nonzero elements would be as depicted in Figure F-3.

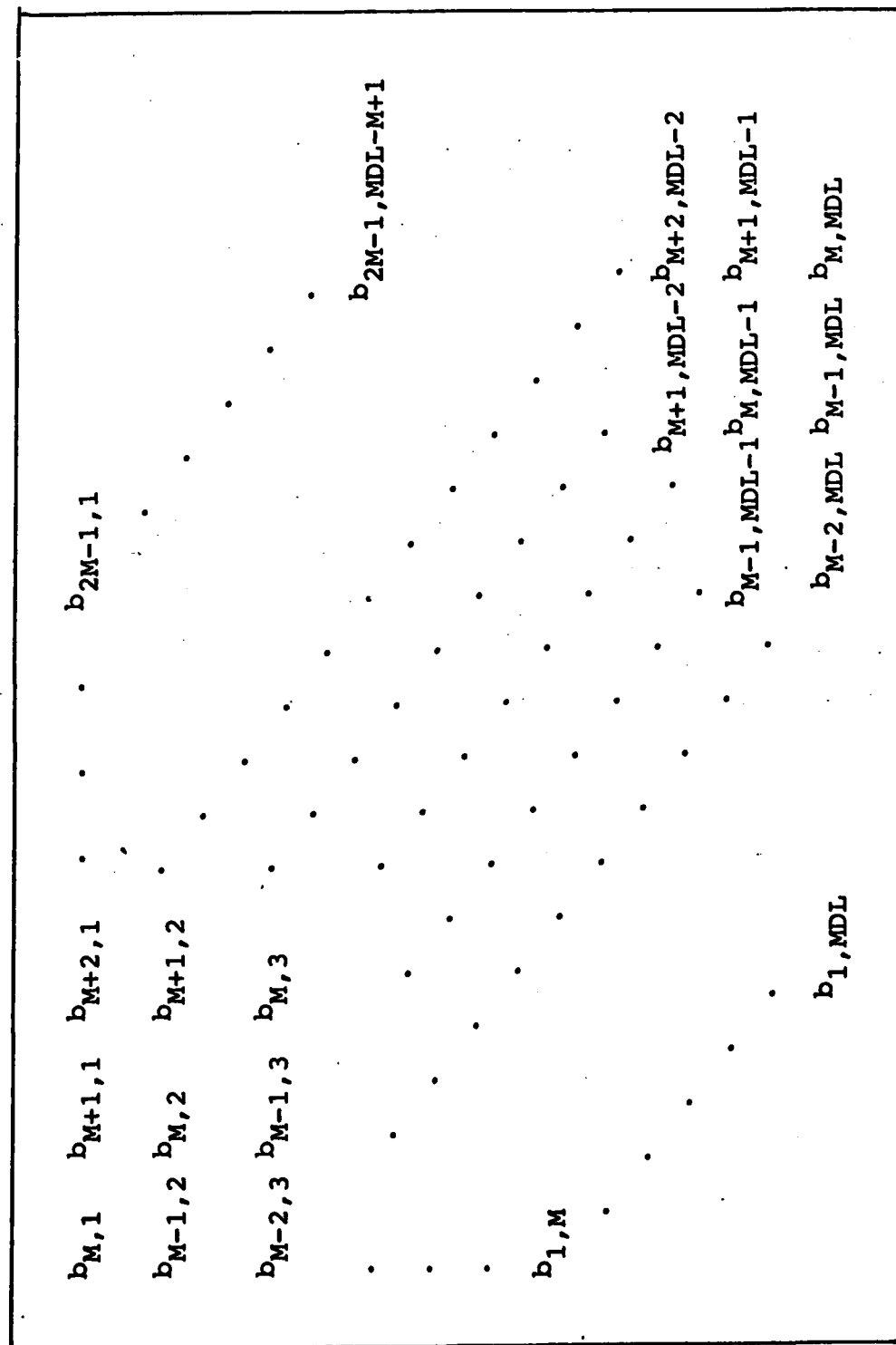


Figure F-4. Generalized Band Stored Coefficient Matrix

VITA

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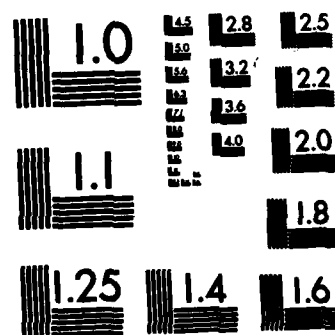
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condition. Oscillatory behavior of the fully explicit FDMTH was as predicted by the general stability condition. Though the Crank-Nicholson implicit and the Peaceman-Rachford ADI FDMTHs were expected to be unconditionally stable, unstable oscillations were observed for large sizes of time step. For large numbers of time steps and sizes of time steps for which all FDMTHs considered are stable, the Crank-Nicholson implicit FDMTH is the more accurate.

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